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Adaptive Finite Element Approximations for a Class of Nonlinear Eigenvalue Problems in Quantum Physics

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Abstract. In this paper, we study an adaptive finite element method for a class of nonlinear eigenvalue problems resulting from quantum physics that may have a nonconvex energy functional. We prove the convergence of adaptive finite element approximations and present several numerical examples of micro-structure of matter calculations that support our theory.

AMS subject classifications: 35Q55, 65N15, 65N25, 65N30, 81Q05

Key words: Adaptive finite element, convergence, micro-structure, nonlinear eigenvalue.

1 Introduction

In this paper, we study adaptive finite element approximations for a class of nonlinear eigenvalue problems: find $(\lambda, u)\in\mathbb{R}\times H_0^1(\Omega)$ such that

$$\begin{cases} \big(-\alpha\Delta + V + \mathcal{N}(u^2)\big)u = \lambda u, & \text{in } \Omega, \\ \displaystyle\int_\Omega |u|^2 = Z, \end{cases} \tag{1.1}$$

where $\Omega\subset\mathbb{R}^3$, $Z\in\mathbb{N}$, $\alpha\in(0,\infty)$, $V:\Omega\to\mathbb{R}$ is a given function, $\mathcal{N}$ maps a nonnegative function over Ω to some function defined on Ω.

Many physical models for micro-structures of matter are nonlinear eigenvalue problems of type (1.1), for instance, the Thomas-Fermi-von Weizsäcker (TFW) type orbital-free model used for electronic structure calculations [15, 31, 41] and the Gross-Pitaevskii equation (GPE) describing the Bose-Einstein condensates (BEC) [4, 42]. In

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the context of simulations of electronic structure calculations, the basis functions used to discretize models like (1.1) are traditionally plane wave bases or typically Gaussian approximations of the eigenfunctions of a hydrogen-like operator. The former is very well adapted to solid state calculations and the latter is incredibly efficient for calculations of molecular systems. However, there are several disadvantages and limitations involved in such methods. For example, the boundary condition does not correspond to that of an actual system; extensive global communications in dealing with plane waves reduce the efficiency of a massive parallelization, which is necessary for complex systems; and the generation of a large supercell is needed for non-periodic systems, which certainly increases the computational cost. The finite element method uses local piecewise polynomial basis functions, which does not involve problems mentioned above and has several advantages. Although it uses more degrees of freedom than that of traditional methods, strictly local basis functions produce well structured sparse Hamiltonian matrices; arbitrary boundary conditions can be easily incorporated; more importantly, since ground state solutions oscillate obviously near the nuclei, it is relatively straightforward to implement adaptive refinement techniques for describing regions around nuclei or chemical bonds where the electron density varies rapidly, while treating the other zones with a coarser description, by which computational accuracy and efficiency can be well controlled. Thus it should be natural to apply adaptive finite element methods to solve nonlinear eigenvalue problems resulting from modeling electronic structures. Indeed the adaptive finite element method is a powerful approach to computing ground state energies and densities in quantum chemistry, materials science, molecular biology and nanosciences [5,30].

The basic idea of a standard adaptive finite element method is to repeat the following procedure until a certain accuracy is obtained:

$$\text{Solve} \rightarrow \text{Estimate} \rightarrow \text{Mark} \rightarrow \text{Refine}.$$

Adaptive finite element methods have been studied extensively since Babuška and Rheinboldt [3] and have been successful in the practice of engineering and scientific computing. In particular, Dörfler [21] presented the first multidimensional convergence result, which has been improved and generalized, see, e.g., [6,8,32–35,38] for linear boundary value problems, [11,16,20,27,28,39] for nonlinear boundary value problems, and [12,18,22–24] for linear eigenvalue problems. To our best knowledge, there has been no work on the convergence of adaptive finite element approximations for nonlinear eigenvalue problems, though some a priori error analyses of finite dimensional Galerkin discretizations for such nonlinear eigenvalue problems have been shown in [9,10,13,29,42,43].

In this paper, we shall present a posteriori error analysis of an adaptive finite element method for a class of nonlinear eigenvalue problems and prove that the adaptive finite element algorithm will produce a sequence of approximations that converge to exact ground state solutions. As an illustration, we shall also report several numerical experiments on electronic structure calculations based on the adaptive finite element discretization [5,15,30], which support our theory. Since the nonlinear term occurs, especially the nonlocal convolution integration part, there are several serious difficulties in the numerical analysis. Moreover, the associated energy functional for this type of problems is usually nonconvex, which particularly brings troubles in convergence analysis. In our analysis, we shall apply some nonlinear functional arguments and special techniques to deal with the local and nonlocal terms carefully.

This paper is organized as follows. In the coming section, we give an overview of the nonlinear eigenvalue problem and provide an analysis for the nonlocal term. In Section 3, we describe the finite element discretization and present an a posteriori error analysis. In Section 4, we design an adaptive finite element algorithm and prove the convergence of the algorithm. In Section 5, we show some numerical results for microstructure computations that support our theory. Finally, we give several concluding remarks.

2 Preliminaries

Let $\Omega\subset\mathbb{R}^3$ be a polytypic bounded domain. We shall use the standard notation for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms and seminorms, see, e.g., [1, 17]. For $p=2$, we denote

$$H^s(\Omega) = W^{s,2}(\Omega) \quad \text{and} \quad H_0^1(\Omega) = \big\{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\big\},$$

where $v|_{\partial\Omega}=0$ is understood in the sense of trace, $\|\cdot\|_{s,\Omega}=\|\cdot\|_{s,2,\Omega}$, and $(\cdot,\cdot)$ is the standard L^2 inner product. The space $H^{-1}(\Omega)$, the dual of $H_0^1(\Omega)$, will also be used. For convenience, the symbol $\lesssim$ will be used in this paper. The notation $A\lesssim B$ means that $A\leq CB$ for some constant C that is independent of mesh parameters. We shall use $\mathscr{P}(p,(c_1,c_2))$ to denote a class of functions that satisfy the growth condition:

$$\mathscr{P}(p,(c_1,c_2)) = \big\{f:\ \exists a_1,a_2 \in \mathbb{R},\ \text{such that}\ c_1t^p + a_1 \leq f(t) \leq c_2t^p + a_2,\ \ \forall\ t \geq 0\big\},$$

with $c_1\in\mathbb{R}$ and $c_2, p\in[0,\infty)$.

The weak form of (1.1) reads as follows: find $(\lambda,u)\in\mathbb{R}\times H_0^1(\Omega)$, such that

$$\begin{cases} \alpha(\nabla u,\nabla v) + (Vu + \mathcal{N}(u^2)u, v) = \lambda(u,v), \quad \forall v \in H_0^1(\Omega), \\ \|u\|_{0,\Omega}^2 = Z. \end{cases} \tag{2.1}$$

We assume that the nonlinear term $\mathcal{N}$ may be split into local and nonlocal parts:

$$\mathcal{N}(\rho) = \mathcal{N}_1(\rho) + \mathcal{N}_2(\rho),$$

where $\rho=u^2$, $\mathcal{N}_1 : [0,\infty)\to\mathbb{R}$ is a given function dominated by some polynomial, and $\mathcal{N}_2$ is represented by a convolution integration

$$\mathcal{N}_2(\rho) = \rho^{q-1}\int_\Omega \rho^q(y)K(\cdot - y)dy,$$

for some given function K and $q\in\mathbb{R}$.

The associated energy functional with respect to this nonlinear eigenvalue problem is expressed by

$$E(u)=\int_\Omega\big(\alpha|\nabla u(x)|^2+V(x)u^2(x)+\mathcal{F}(u^2(x))\big)dx+\frac{1}{2q}D_K(u^{2q},u^{2q}), \tag{2.2}$$

where $\mathcal{F}:[0,\infty)\to\mathbb{R}$ is associated with $\mathcal{N}_1$:

$$\mathcal{F}(s)=\int_0^s\mathcal{N}_1(t)dt,$$

and $D_K(\cdot,\cdot)$ is a bilinear form defined by

$$D_K(f,g)=\int_\Omega\int_\Omega f(x)g(y)K(x-y)dxdy.$$

Remark 2.1. In the orbital-free model for electronic structure calculation [15, 41], the first term in energy functional (2.2) represents von Weizsäcker kinetic energy, the second term is the interaction energy with the external potential V, the third term denotes the Thomas-Fermi kinetic energy and exchange-correction energy, and the last term is the electrostatic interaction energy of electrons and the nonlocal kinetic energy.

The ground state solution of problem (1.1) is obtained by minimizing energy functional (2.2) in the admissible class

$$\mathcal{A}=\big\{\psi\in H_0^1(\Omega):\ \|\psi\|_{0,\Omega}^2=Z,\ \ \psi\geq 0\big\}.$$

In our discussion, we assume that

(i) $V\in L^2(\Omega)$.

(ii) $\mathcal{F}\in\mathscr{P}(p,(c_1,c_2))$ with one of the following conditions:

1. $c_1\in(0,\infty)$;
2. $p\in[0,4/3]$;
3. $c_1\in(-\infty,0)$, $p\in(4/3,\infty)$ and

$$\frac{|c_1|}{\alpha}Z^{p-1}<\inf_{\substack{u\in H_0^1(\Omega)\\ \|u\|_{0,\Omega}=1}}\frac{\int_\Omega|\nabla u|^2}{\int_\Omega|u|^{2p}}. \tag{2.3}$$

(iii) $\mathcal{N}_1(t)\in\mathscr{P}(p_1,(c_1,c_2))$ for some $p_1\in[0,2)$ and $t\mathcal{N}_1'(t)\in\mathscr{P}(p_2,(\tilde{c}_1,\tilde{c}_2))$ for some $p_2\in[0,2)$.

(iv) $K\in L^2(\tilde{\Omega})$, where $\tilde{\Omega}=\{x-y: x,y\in\Omega\}$. Moreover, K is some nonnegative even function and $q\in[1,3/2)$.

Note that these assumptions are satisfied by typical physical models for micro-structures of matter (see, e.g., [7, 15, 19, 30, 31]) and condition (2.3) first appeared in [7].

It is known that under Assumptions (i)-(iv), there exists a nonnegative minimizer of energy functional (2.2) [13, 31, 43]. Moreover, $E(v)$ is bounded below over $\mathcal{A}$ under these assumptions [13, 43], namely, there exist positive constants C and b such that

$$E(v) \geq C^{-1}\|\nabla v\|_{0,\Omega}^2 - b, \quad \forall v \in \mathcal{A}. \tag{2.4}$$

In general, however, the uniqueness of the nonnegative ground state solution is unknown, of which the main reason is that energy functional (2.2) is nonconvex with respect to $\rho = u^2$ for almost all molecular models of practical interest. As a result, we introduce the set of ground state solutions by

$$\mathcal{U} = \big\{u \in \mathcal{A} : E(u) = \min_{v \in \mathcal{A}} E(v)\big\}. \tag{2.5}$$

If $u \in \mathcal{U}$ is a ground state solution, then there exists a corresponding Lagrange multiplier $\lambda \in \mathbb{R}$ such that (λ, u) solves (2.1) and satisfies

$$Z\lambda = E(u) + \int_\Omega \big(\mathcal{N}_1(u^2(x))u^2(x) - \mathcal{F}(u^2(x))\big)dx + \Big(1 - \frac{1}{2q}\Big)D_K(u^{2q}, u^{2q}).$$

We define the set of ground state eigenvalues by

$$\Lambda = \big\{\lambda \in \mathbb{R} : (\lambda, u) \text{ solves (2.1)}, \ u \in \mathcal{U}\big\}.$$

The following estimate of the nonlinear term will be used in our analysis.

Lemma 2.1. *Let $\chi, w \in H^1(\Omega)$ satisfy*

$$\|\chi\|_{1,\Omega} + \|w\|_{1,\Omega} \leq \bar{C},$$

for some constant $\bar{C}$. If the Assumptions (iii) *and* (iv) *are satisfied, then there exists a constant $\widetilde{C} > 0$ depending on $\bar{C}$, the volume of Ω and constants and parameters involved in Assumptions* (iii) *and* (iv) *such that*

$$\int_\Omega \big(\mathcal{N}(\chi^2)\chi - \mathcal{N}(w^2)w\big)v \leq \widetilde{C}\|\chi - w\|_{1,\Omega}\|v\|_{1,\Omega}, \quad \forall v \in H_0^1(\Omega). \tag{2.6}$$

Proof. We first prove that

$$\int_\Omega \big(\mathcal{N}_1(\chi^2)\chi - \mathcal{N}_1(w^2)w\big)v \lesssim \|\chi - w\|_{1,\Omega}\|v\|_{1,\Omega}, \quad \forall v \in H_0^1(\Omega), \tag{2.7}$$

which is valid when $p_1, p_2 \in (0, 2)$ in Assumption (iii). For $p_1, p_2 \in (0, 2)$, there exists $\xi = \chi + \delta(w - \chi)$ with $\delta \in [0, 1]$, such that

$$\begin{aligned}
&\int_\Omega \big(\mathcal{N}_1(\chi^2)\chi - \mathcal{N}_1(w^2)w\big)v \\
=&\int_\Omega \big(\mathcal{N}_1(\xi^2) + 2\xi^2\mathcal{N}_1'(\xi^2)\big)(\chi - w)v \\
\leq&\|\mathcal{N}_1(\xi^2)\|_{0,\frac{3}{p_1},\Omega}\|\chi - w\|_{0,\frac{6}{5-2p_1},\Omega}\|v\|_{0,6,\Omega} \\
&+ \|2\xi^2\mathcal{N}_1'(\xi^2)\|_{0,\frac{3}{p_2},\Omega}\|\chi - w\|_{0,\frac{6}{5-2p_2},\Omega}\|v\|_{0,6,\Omega}.
\end{aligned} \tag{2.8}$$

From Assumption (iii), there exist constants $a_1, a_2, \widetilde{a}_1$ and $\widetilde{a}_2$ such that

$$a_1 + c_1\xi^{2p_1} \le \mathcal{N}_1(\xi^2) \le a_2 + c_2\xi^{2p_1}, \tag{2.9a}$$

$$\widetilde{a}_1 + \widetilde{c}_1\xi^{2p_2} \le \xi^2\mathcal{N}_1'(\xi^2) \le \widetilde{a}_2 + \widetilde{c}_2\xi^{2p_2}, \tag{2.9b}$$

which together with (2.8) and the Sobolev inequality imply

$$\begin{aligned}\int_\Omega \big(\mathcal{N}_1(\chi^2)\chi - \mathcal{N}_1(w^2)w\big)v \le& \Big(a_2|\Omega|^{\frac{p_1}{3}} + c_2\|\xi^{2p_1}\|_{0,\frac{3}{p_1},\Omega}\Big)\|\chi - w\|_{1,\Omega}\|v\|_{1,\Omega} \\ &+ \Big(2\widetilde{a}_2|\Omega|^{\frac{p_2}{3}} + 2\widetilde{c}_2\|\xi^{2p_2}\|_{0,\frac{3}{p_2},\Omega}\Big)\|\chi - w\|_{1,\Omega}\|v\|_{1,\Omega},\end{aligned}$$

where $|\Omega|$ is the volume of Ω. Note that

$$\|\xi\|_{0,6,\Omega} \lesssim \|\chi\|_{0,6,\Omega} + \|w\|_{0,6,\Omega} \lesssim \|\chi\|_{1,\Omega} + \|w\|_{1,\Omega} \le \bar{C},$$

we get that (2.7) holds for $p_1, p_2 \in (0,2)$. Similar arguments show that (2.7) is also true when $p_1p_2=0$.

For nonlocal term $\mathcal{N}_2$, we obtain from Assumption (iv), the Young's inequality, and the Hölder inequality that

$$\begin{aligned}\|K*(\chi^{2q} - w^{2q})\|_{0,\infty,\Omega} \lesssim& \|K\|_{0,\widetilde{\Omega}}\|\chi^{2q} - w^{2q}\|_{0,\Omega} \\ \lesssim& \|K\|_{0,\widetilde{\Omega}}\|\xi^{2q-1}\|_{0,\frac{6}{5},\Omega}\|\chi - w\|_{0,6,\Omega} \\ \lesssim& \|\chi - w\|_{1,\Omega}.\end{aligned}$$

Hence, for all $v \in H_0^1(\Omega)$, we have

$$\begin{aligned}\int_\Omega K*(\chi^{2q} - w^{2q})\chi^{2q-1}v \lesssim& \|K*(\chi^{2q} - w^{2q})\|_{0,\infty,\Omega}\|\chi^{2q-1}\|_{0,\Omega}\|v\|_{0,\Omega} \\ \lesssim& \|\chi - w\|_{1,\Omega}\|\chi\|^{2q-1}_{0,2(2q-1),\Omega}\|v\|_{0,\Omega} \\ \lesssim& \|\chi - w\|_{1,\Omega}\|v\|_{1,\Omega},\end{aligned} \tag{2.10}$$

where $q \in [1, 3/2)$ as in Assumption (iv). Similarly, for all $v \in H_0^1(\Omega)$, there holds

$$\begin{aligned}\int_\Omega K*w^{2q}(\chi^{2q-1} - w^{2q-1})v \lesssim& \|K*w^{2q}\|_{0,\infty,\Omega}\|\chi^{2q-1} - w^{2q-1}\|_{0,\Omega}\|v\|_{0,\Omega} \\ \lesssim& \|\xi^{2q-2}\|_{0,\frac{3}{q-1},\Omega}\|\chi - w\|_{0,\frac{6}{5-2q},\Omega}\|v\|_{1,\Omega} \\ \lesssim& \|\chi - w\|_{1,\Omega}\|v\|_{1,\Omega}.\end{aligned} \tag{2.11}$$

Taking (2.10), (2.11), and identity

$$\mathcal{N}_2(\chi^2)\chi - \mathcal{N}_2(w^2)w = K*(\chi^{2q} - w^{2q})\chi^{2q-1} + K*w^{2q}(\chi^{2q-1} - w^{2q-1}),$$

into account, we obtain

$$\int_\Omega \big(\mathcal{N}_2(\chi^2)\chi - \mathcal{N}_2(w^2)w\big)v \lesssim \|\chi - w\|_{1,\Omega}\|v\|_{1,\Omega}, \quad \forall v \in H_0^1(\Omega),$$

which together with (2.7) leads to (2.6). This completes the proof. $\square$

3 Finite element discretizations

Let d_Ω be the diameter of Ω and $\{\mathcal{T}_h\}$ be a shape regular family of nested conforming meshes over Ω with size $h\in(0,d_\Omega)$: there exists a constant γ^* such that

$$\frac{h_T}{\rho_T}\le\gamma^*,\quad \forall T\in\mathcal{T}_h,$$

where, for each $T\in\mathcal{T}_h$, h_T is the diameter of T, ρ_T is the diameter of the biggest ball contained in T, and $h=\max\{h_T : T\in\mathcal{T}_h\}$. Let $\mathcal{E}_h$ denote the set of interior faces of $\mathcal{T}_h$. And we shall also use a slightly abused of notation that h denotes the mesh size function defined by

$$h(x)=h_T,\quad x\in T,\quad \forall T\in\mathcal{T}_h.$$

Let $S^h(\Omega)\subset H^1(\Omega)$ be a corresponding family of nested finite element spaces consisting of continuous piecewise polynomials over $\mathcal{T}_h$ of fixed degree $n\ge1$ and

$$S^h_0(\Omega)=S^h(\Omega)\cap H^1_0(\Omega).$$

Set

$$\mathcal{V}_h=S^h_0(\Omega)\cap\mathcal{A}.$$

Under Assumptions (i)-(iv), we can obtain the existence of nonnegative ground state solutions in $\mathcal{V}_h$ (see, e.g., [43]). We do not have any uniqueness result for this discrete problem since the energy functional and the admissible set are nonconvex. We define the set of ground state solutions in $\mathcal{V}_h$ by

$$\mathcal{U}_h=\big\{u_h\in\mathcal{V}_h : E(u_h)=\min_{v\in\mathcal{V}_h}E(v)\big\}. \tag{3.1}$$

We have from (2.4) that $\|u_h\|_{1,\Omega}$ is uniformly bounded

$$\sup_{\substack{h\in(0,d_\Omega)\\ u_h\in\mathcal{U}_h}}\|u_h\|_{1,\Omega}\le C, \tag{3.2}$$

with some constant C.

It is seen that a minimizer $u_h\in\mathcal{U}_h$ solves

$$\begin{cases}\alpha(\nabla u_h,\nabla v)+(Vu_h+\mathcal{N}(u_h^2)u_h,v)=\lambda_h(u_h,v), & \forall v\in S^h_0(\Omega),\\ \|u_h\|^2_{0,\Omega}=Z,\end{cases} \tag{3.3}$$

with the corresponding finite element eigenvalue $\lambda_h\in\mathbb{R}$ satisfying

$$Z\lambda_h=E(u_h)+\int_\Omega\big(\mathcal{N}_1(u_h^2(x))u_h^2(x)-\mathcal{F}(u_h^2(x))\big)dx+\Big(1-\frac{1}{2q}\Big)D_K(u_h^{2q},u_h^{2q}). \tag{3.4}$$

Define

$$\Lambda_h=\big\{\lambda_h\in\mathbb{R} : (\lambda_h,u_h)\text{ solves (3.3)},\ u_h\in\mathcal{U}_h\big\}.$$

A priori error analysis for (3.3) has been shown in [13]. To carry out a posteriori error analysis, we need the following result.

Lemma 3.1. *If the Assumptions* (iii) *and* (iv) *are satisfied, then there holds*

$$h_T\|\mathcal{N}(u_h^2)u_h\|_{0,T} \lesssim \|u_h\|_{0,6,T}, \quad \forall T \in \mathcal{T}_h, \tag{3.5}$$

where the hidden constant depends on the volume of T, the constant involved in (3.2) *and constants and parameters involved in Assumptions* (iii) *and* (iv).

Proof. It is obvious that

$$h_T\|\mathcal{N}_1(u_h^2)u_h\|_{0,T} \lesssim \|u_h\|_{0,6,T},$$

holds for $p_1=0$ in Assumption (iii). By (2.9a) and (3.2), the Hölder inequality and the inverse inequality, we have

$$\begin{aligned} h_T\|\mathcal{N}_1(u_h^2)u_h\|_{0,T} \le & h_T\|\mathcal{N}_1(u_h^2)\|_{0,3,T}\|u_h\|_{0,6,T} \\ \le & h_T\big(a_2|T|^{\frac{1}{3}} + c_2\|u_h\|_{0,6p_1,T}^{2p_1}\big)\|u_h\|_{0,6,T} \\ \lesssim & h_T\|u_h\|_{0,6,T} + h_T^{2-p_1}\|u_h\|_{0,6,T}^{2p_1+1}, \end{aligned}$$

for $p_1\in[1,2)$ and

$$h_T\|\mathcal{N}_1(u_h^2)u_h\|_{0,T} \le h_T\big(a_2|T|^{\frac{p_1}{3}} + c_2\|u_h^{2p_1}\|_{0,\frac{3}{p_1},T}\big)\|u_h\|_{0,\frac{6}{3-2p_1},T} \lesssim \|u_h\|_{0,6,T},$$

for $p_1\in(0,1)$. Combining with the estimate of $\mathcal{N}_2$ as follows

$$\begin{aligned} h_T\|\mathcal{N}_2(u_h^2)u_h\|_{0,T} \lesssim & h_T\|K * u_h^{2q}\|_{0,\infty,T}\|u_h^{2q-1}\|_{0,T} \\ \lesssim & h_T\|K\|_{0,\tilde{\Omega}}\|u_h^{2q}\|_{0,\Omega}\|u_h\|_{0,6,T}^{2q-1} \\ \lesssim & \|u_h\|_{0,6,T}, \end{aligned}$$

where Assumption (iv) is used, we obtain (3.5). This completes the proof. □

Let $\mathbb{T}$ denote the class of all conforming refinements by the bisection of an initial triangulation $\mathcal{T}_0$. For $\mathcal{T}_h\in\mathbb{T}$ and any $u_h\in\mathcal{U}_h$ we define element residual $\mathcal{R}_T(u_h)$ and jump residual $J_e(u_h)$ by

$$\begin{aligned} &\mathcal{R}_T(u_h) = \lambda_h u_h + \alpha\Delta u_h - Vu_h - \mathcal{N}(u_h^2)u_h, && \text{in } T \in \mathcal{T}_h, \\ &J_e(u_h) = \alpha\nabla u_h|_{T_1}\cdot\overrightarrow{n_1} + \alpha\nabla u_h|_{T_2}\cdot\overrightarrow{n_2} = \alpha[[\nabla u_h]]_e\cdot\overrightarrow{n_1}, && \text{on } e \in \mathcal{E}_h, \end{aligned}$$

where T_1 and T_2 are elements in $\mathcal{T}_h$ which share e and $\overrightarrow{n_i}$ is the outward normal vector of T_i on e for i=1,2. Let $\omega_h(e)$ be the union of elements which share e and $\omega_h(T)$ be the union of elements sharing a side with T.

For $T\in\mathcal{T}_h$, we define local error indicator $\eta_h(u_h,T)$ by

$$\eta_h^2(u_h,T) = h_T^2\|\mathcal{R}_T(u_h)\|_{0,T}^2 + \sum_{\substack{e\in\mathcal{E}_h \\ e\subset\partial T}} h_e\|J_e(u_h)\|_{0,e}^2. \tag{3.6}$$

Given a subset $\omega\subset\Omega$, we define error estimator $\eta_h(u_h,\omega)$ by

$$\eta_h^2(u_h,\omega)=\sum_{\substack{T\in\mathcal{T}_h\\ T\subset\omega}}\eta_h^2(u_h,T).$$

The following result will be used in our convergence analysis though it looks rough.

Proposition 3.1. *Let $\mathcal{T}_h\in\mathbb{T}$ and (λ_h,u_h) be a solution of* (3.3). *If Assumptions* (i)-(iv) *are satisfied, then*

$$\eta_h(u_h,T)\lesssim\|u_h\|_{0,6,\omega_h(T)}+\|u_h\|_{1,\omega_h(T)},\quad\forall T\in\mathcal{T}_h,$$

and

$$\eta_h(u_h,\Omega)\le C_\eta,$$

where the uniform constant $C_\eta>0$ is independent of the mesh size h.

Proof. We first analyze the element residual. From the boundness of λ_h, we have

$$\begin{aligned}h_T\|\mathcal{R}_T(u_h)\|_{0,T}=&h_T\|\lambda_hu_h+\alpha\Delta u_h-Vu_h-\mathcal{N}(u_h^2)u_h\|_{0,T}\\ \lesssim&h_T\|u_h\|_{0,T}+h_T\|\Delta u_h\|_{0,T}+h_T\|Vu_h\|_{0,T}+h_T\|\mathcal{N}(u_h^2)u_h\|_{0,T}.\end{aligned}$$

Using the inverse inequality, Assumption (i) and Lemma 3.1, we have

$$h_T\|\mathcal{R}_T(u_h)\|_{0,T}\lesssim\|u_h\|_{0,6,T}+\|u_h\|_{1,T},$$

to which similar estimates are true when T is replaced by any $T'\in\omega_h(T)$.

For the jump residual, we derive from the definition of $J_e(u_h)$ and the inverse inequality that

$$\begin{aligned}h_e^{\frac12}\|J_e(u_h)\|_{0,e}=&h_e^{\frac12}\|\alpha\nabla u_h|_{T_1}\cdot\overrightarrow{n_1}+\alpha\nabla u_h|_{T_2}\cdot\overrightarrow{n_2}\|_{0,e}\\ \lesssim&h_e^{\frac12}\left(\|\nabla u_h|_{T_1}\|_{0,e}+\|\nabla u_h|_{T_2}\|_{0,e}\right)\\ \lesssim&\|u_h\|_{1,\omega_h(T)}.\end{aligned}$$

Consequently, we get

$$\sum_{\substack{e\in\mathcal{E}_h\\ e\subset\partial T}}h_e^{\frac12}\|J_e(u_h)\|_{0,e}\lesssim\|u_h\|_{1,\omega_h(T)}.$$

From (3.2), the definition of $\eta_h(u_h,T)$ and $\eta_h(u_h,\Omega)$, we then finish the proof. $\Box$

To present upper and lower error bounds, we introduce an oscillation $osc_h(u_h,T)$ for any $T\in\mathcal{T}_h$ by

$$\mathrm{osc}_h^2(u_h,T)=h_T^2\big\|\mathcal{R}_T(u_h)-\overline{\mathcal{R}_T(u_h)}\big\|_{0,T}^2,$$

where $\overline{\mathcal{R}_T(u_h)}\in P_{n-1}$ denotes the L^2 projection of $\mathcal{R}_T(u_h)$. For a subset $\omega\subset\Omega$, we define

$$\mathrm{osc}_h^2(u_h,\omega)=\sum_{\substack{T\in\mathcal{T}_h\\ T\subset\omega}}\mathrm{osc}_h^2(u_h,T).$$

We have from a standard argument that (see Appendix for a proof).

Theorem 3.1. *Let (λ,u) be a regular ground state solution of* (2.1). *If (λ_h,u_h) is sufficiently close to (λ,u), then*

$$\eta_h(u_h,\Omega)-\mathrm{osc}_h(u_h,\Omega)\lesssim|\lambda-\lambda_h|+\|u-u_h\|_{1,\Omega}\lesssim\eta_h(u_h,\Omega)+\mathrm{osc}_h(u_h,\Omega).$$

Remark 3.1. The definition of a regular ground state solution is referred to the Appendix. Theorem 3.1 provides the standard upper and lower bounds of the error with respect to the error estimator. However, the hypothesis that (λ,u) is a regular solution is somehow strong, which can not be proved for most of the problems of practical interest (c.f., e.g., Appendix). Anyway, it will not be used in our convergence analysis.

We define the global residual $\mathbf{R}_h(u_h)\in H^{-1}(\Omega)$ as follows

$$\langle\mathbf{R}_h(u_h),v\rangle=\lambda_h(u_h,v)-(\alpha\nabla u_h,\nabla v)-(Vu_h,v)-(\mathcal{N}(u_h^2)u_h,v),\quad\forall v\in H_0^1(\Omega),\tag{3.7}$$

and see that

$$\langle\mathbf{R}_h(u_h),v\rangle=\sum_{T\in\mathcal{T}_h}\Big(\int_T\mathcal{R}_T(u_h)v-\sum_{\substack{e\in\mathcal{E}_h\\ e\subset\partial T}}\int_e J_e(u_h)v\Big),\quad\forall v\in H_0^1(\Omega).$$

The global residual can be estimated by the local error indicators in the following sense.

Theorem 3.2. *If $(\lambda_h,u_h)\in\mathbb{R}\times\mathcal{V}_h$ is a solution of* (3.3), *then*

$$|\langle\mathbf{R}_h(u_h),v\rangle|\lesssim\sum_{T\in\mathcal{T}_h}\eta_h(u_h,T)\|v\|_{1,\omega_h(T)},\quad\forall v\in H_0^1(\Omega).$$

Proof. Let $v\in H_0^1(\Omega)$ and $v_h\in S_0^h(\Omega)$ be the Clément interpolant of v satisfying

$$\|v-v_h\|_{0,T}\lesssim h_T\|\nabla v\|_{0,\omega_h(T)}\quad\text{and}\quad\|v-v_h\|_{0,\partial T}\lesssim h_T^{\frac{1}{2}}\|\nabla v\|_{0,\omega_h(T)}.$$

Due to (3.7) and the fact $\langle\mathbf{R}_h(u_h),v_h\rangle=0$, we obtain

$$\begin{aligned}
&|\langle\mathbf{R}_h(u_h),v\rangle|=|\langle\mathbf{R}_h(u_h),v-v_h\rangle|\\
\le&\sum_{T\in\mathcal{T}_h}\Big(\|\mathcal{R}_T(u_h)\|_{0,T}\|v-v_h\|_{0,T}+\sum_{\substack{e\in\mathcal{E}_h\\ e\subset\partial T}}\|J_e(u_h)\|_{0,e}\|v-v_h\|_{0,e}\Big)\\
\lesssim&\sum_{T\in\mathcal{T}_h}\Big(\|h\mathcal{R}_T(u_h)\|_{0,T}\|v\|_{1,\omega_h(T)}+\sum_{\substack{e\in\mathcal{E}_h\\ e\subset\partial T}}\|h^{\frac{1}{2}}J_e(u_h)\|_{0,e}\|v\|_{1,\omega_h(T)}\Big)\\
\lesssim&\sum_{T\in\mathcal{T}_h}\eta_h(u_h,T)\|v\|_{1,\omega_h(T)}.
\end{aligned}$$

This completes the proof. $\square$

4 Convergence of adaptive finite element computations

We shall first recall the adaptive finite element algorithm. For convenience, we shall replace the subscript h (or h_k) by an iteration counter k of the adaptive algorithm afterwards. Given an initial triangulation $\mathcal{T}_0$, we can generate a sequence of nested conforming triangulations $\mathcal{T}_k$ using the following loop:

$$\text{Solve} \rightarrow \text{Estimate} \rightarrow \text{ Mark} \rightarrow \text{Refine.}$$

More precisely, to get $\mathcal{T}_{k+1}$ from $\mathcal{T}_k$ we first solve the discrete problem (3.1) to get $\mathcal{U}_k$ on $\mathcal{T}_k$. The error is estimated by any $u_k \in \mathcal{U}_k$ and used to mark a set of elements that are to be refined. Elements are refined in such a way that the triangulation is still shape regular and conforming.

Here, we shall not discuss the step "Solve", which deserves a separate investigation. We assume that solutions of finite dimensional problems can be solved to any accuracy efficiently. The procedure "Estimate" determines the element indicators for all elements $T \in \mathcal{T}_k$. A posteriori error estimators are an essential part of this step, which have been investigated in the previous section. In the following discussion, we use $\eta_k(u_k, T)$ defined by (3.6) as the a posteriori error estimator. Depending on the relative size of the element indicators, these quantities are later used by the procedure "Mark" to mark elements in $\mathcal{T}_k$ and thereby create a subset of elements to be refined. The only requirement we make on this step is that the set of marked elements $\mathcal{M}_k$ contains at least one element of $\mathcal{T}_k$ holding the largest value estimator [22, 23]. Namely, there exists one element $T_k^{\max} \in \mathcal{M}_k$ such that

$$\eta_k(u_k, T_k^{\max}) = \max_{T \in \mathcal{T}_k} \eta_k(u_k, T). \tag{4.1}$$

It is easy to check that the most commonly used marking strategies, e.g., Maximum strategy, Equidistribution strategy, and Dörfler's strategy fulfill this condition. Finally, the marked elements are refined to force the error reduction by the procedure "Refine". The basic algorithm in this step is the tetrahedral bisection, with the data structure named marked tetrahedron, the tetrahedra are classified into 5 types and the selection of refinement edges depends only on the type and the ordering of vertices for the tetrahedra [2]. Note that a few more elements $T \in \mathcal{T}_k \backslash \mathcal{M}_k$ are partitioned to maintain mesh conformity. It is worth mentioning that we do not assume to enforce the so-called interior node property.

The adaptive finite element algorithm without oscillation marking is stated as follows:

Algorithm 4.1.

1. Pick any initial mesh $\mathcal{T}_0$, and let $k = 0$.
2. Solve the system on $\mathcal{T}_k$ to get discrete solutions $(\Lambda_k, \mathcal{U}_k)$.
3. Choose any $u_k \in \mathcal{U}_k$ and compute local error indictors $\eta_k(u_k, T)$, $\forall T \in \mathcal{T}_k$.

4. Construct $\mathcal{M}_k \subset \mathcal{T}_k$ by a marking strategy that satisfies (4.1).
5. Refine $\mathcal{T}_k$ to get a new conforming mesh $\mathcal{T}_{k+1}$.
6. Let $k = k+1$ and go to 2.

The purpose of this paper is to prove that Algorithm 4.1 generates a sequence of adaptive finite element solutions which converge to some ground state solutions of (2.5). More precisely, we shall prove that

$$\lim_{k\to\infty} \mathrm{dist}_{H^1}(\mathcal{U}_k,\mathcal{U}) = 0, \qquad \lim_{k\to\infty} \mathrm{dist}(\Lambda_k,\Lambda) = 0,$$

where

$$\mathrm{dist}_{H^1}(F,G) = \sup_{f\in F} \inf_{g\in G} \|f-g\|_{1,\Omega},$$

for any $F,G\subset H^1(\Omega)$, and

$$\mathrm{dist}(A,B) = \sup_{a\in A} \inf_{b\in B} |a-b|,$$

for any $A,B\subset\mathbb{R}$.

We first show that the adaptive finite element approximations are convergent. Given an initial mesh $\mathcal{T}_0$, Algorithm 4.1 generates a sequence of meshes $\mathcal{T}_1,\mathcal{T}_2,\cdots$, and associated discrete subspaces

$$S_0^{h_0}(\Omega) \subsetneq S_0^{h_1}(\Omega) \subsetneq \cdots \subsetneq S_0^{h_n}(\Omega) \subsetneq S_0^{h_{n+1}}(\Omega) \subsetneq \cdots \subsetneq S_\infty(\Omega) \subseteq H_0^1(\Omega),$$

where

$$S_\infty(\Omega) = \overline{\cup S_0^{h_k}(\Omega)}^{H_0^1(\Omega)}.$$

It is obvious that $S_\infty(\Omega)$ is a Hilbert space with the inner product inherited from $H_0^1(\Omega)$, and there holds

$$\lim_{k\to\infty} \inf_{v_k\in S_0^{h_k}(\Omega)} \|v_k - v_\infty\|_{1,\Omega} = 0, \quad \forall v_\infty \in S_\infty(\Omega). \tag{4.2}$$

We set

$$\mathcal{V}_\infty = S_\infty(\Omega) \cap \mathcal{A}.$$

Under Assumptions (i)-(iv), the existence of minimizers of energy functional (2.2) in $\mathcal{V}_\infty$ can be obtained. Similar to (2.5) and (3.1), we introduce the set of minimizers by

$$\mathcal{U}_\infty = \big\{u\in\mathcal{V}_\infty : E(u) = \min_{v\in\mathcal{V}_\infty} E(v)\big\}.$$

We see that $u_\infty \in \mathcal{U}_\infty$ solves

$$\begin{cases} \alpha(\nabla u_\infty,\nabla v) + (Vu_\infty + \mathcal{N}(u_\infty^2)u_\infty, v) = \lambda_\infty(u_\infty, v), & \forall v\in S_\infty(\Omega), \\ \|u_\infty\|_{0,\Omega}^2 = Z, \end{cases} \tag{4.3}$$

with the corresponding eigenvalue $\lambda_\infty \in \mathbb{R}$ satisfying

$$Z\lambda_\infty = E(u_\infty) + \int_\Omega \big(\mathcal{N}_1(u_\infty^2(x))u_\infty^2(x) - \mathcal{F}(u_\infty^2(x))\big)dx + \Big(1 - \frac{1}{2q}\Big)D_K(u_\infty^{2q}, u_\infty^{2q}), \tag{4.4}$$

and we define

$$\Lambda_\infty = \big\{\lambda_\infty \in \mathbb{R} : (\lambda_\infty, u_\infty) \text{ solves (4.3)},\ u_\infty \in \mathcal{U}_\infty\big\}.$$

Theorem 4.1. *If $\{\mathcal{U}_k\}_{k\in\mathbb{N}}$ is the sequence of adaptive finite element approximations generated by Algorithm* 4.1, *then*

$$\lim_{k\to\infty} E_k = \min_{v\in V_\infty} E(v), \qquad \lim_{k\to\infty} \mathrm{dist}_{H^1}(\mathcal{U}_k, \mathcal{U}_\infty) = 0,$$

where

$$E_k = E(v)(v \in \mathcal{U}_k).$$

Moreover, there holds

$$\lim_{k\to\infty} \mathrm{dist}(\Lambda_k, \Lambda_\infty) = 0.$$

Proof. Following [42, 43] (see also [13]), let $u_k \in \mathcal{U}_k$ be such that (λ_k, u_k) solves (3.3) in $\mathbb{R} \times \mathcal{V}_k$ for $k=1,2,\cdots$, and $\{u_{k_m}\}_{m\in\mathbb{N}}$ be any subsequence of $\{u_k\}_{k\in\mathbb{N}}$ with $1 \le k_1 < k_2 < \cdots < k_m < \cdots$.

Note that (3.2) and the Banach-Alaoglu Theorem yield that there exists a weakly convergent subsequence $\{u_{k_{m_j}}\}_{j\in\mathbb{N}}$ and $u_\infty \in S_\infty(\Omega)$ satisfying

$$u_{k_{m_j}} \rightharpoonup u_\infty, \quad \text{in } H_0^1(\Omega), \tag{4.5}$$

we need only to prove

$$E(u_\infty) = \min_{v\in V_\infty} E(v), \tag{4.6a}$$

$$\lim_{j\to\infty} \|u_{k_{m_j}} - u_\infty\|_{1,\Omega} = 0, \tag{4.6b}$$

$$\lim_{j\to\infty} |\lambda_{k_{m_j}} - \lambda_\infty| = 0, \tag{4.6c}$$

where $(\lambda_{k_{m_j}}, u_{k_{m_j}})$ solves (3.3) and $(\lambda_\infty, u_\infty)$ solves (4.3).

Since $H_0^1(\Omega)$ is compactly imbedded in $L^p(\Omega)$ for $p \in [2,6)$, by passing to a further subsequence, we may assume that $u_{k_{m_j}} \to u_\infty$ strongly in $L^p(\Omega)$ as $j \to \infty$. Thus we can derive

$$\lim_{j\to\infty} \int_\Omega \mathcal{F}(u_{k_{m_j}}^2) = \int_\Omega \mathcal{F}(u_\infty^2),$$

$$\lim_{j\to\infty} D_K(u_{k_{m_j}}^{2q}, u_{k_{m_j}}^{2q}) = D_K(u_\infty^{2q}, u_\infty^{2q}),$$

and hence

$$\liminf_{j\to\infty} E(u_{k_{m_j}}) \geq E(u_\infty). \tag{4.7}$$

Note that (4.2) implies that $\{u_{k_{m_j}}\}$ is a minimizing sequence for the energy functional in $S_\infty(\Omega)$, which together with (4.7) and the fact that $\{u_{k_{m_j}}\}$ converge to u_∞ strongly in $L^2(\Omega)$ leads to $u_\infty \in \mathcal{U}_\infty$, namely,

$$\lim_{j\to\infty} E(u_{k_{m_j}}) = E(u_\infty) = \min_{v\in V_\infty} E(v).$$

Consequently, we obtain that each term of $E(v)$ converges and in particular

$$\lim_{j\to\infty} \|\nabla u_{k_{m_j}}\|_{0,\Omega} = \|\nabla u_\infty\|_{0,\Omega}.$$

Using (4.5) and the fact that $H_0^1(\Omega)$ is a Hilbert space under norm $\|\nabla\cdot\|_{0,\Omega}$, we have

$$\lim_{j\to\infty} \|\nabla(u_{k_{m_j}} - u_\infty)\|_{0,\Omega} = 0,$$

which implies (4.6b)

Using (3.4), (4.4), (4.6a) and (4.6b), we immediately obtain (4.6c). This completes the proof. $\square$

Following the ideas in [22,23,35,37], we then prove the convergence of the a posteriori error estimators and the weak convergence of residual $\mathbf{R}_k(u_k)$, which will be used to prove that the adaptive finite element approximations converge to the ground state solutions. Given the sequence $\{\mathcal{T}_k\}_{k\in\mathbb{N}}$, for each $k\in\mathbb{N}$, we define

$$\mathcal{T}_k^+ = \{T \in \mathcal{T}_k : T \in \mathcal{T}_l,\ \forall l \geq k\} \quad \text{and} \quad \mathcal{T}_k^0 = \mathcal{T}_k \setminus \mathcal{T}_k^+.$$

Namely, $\mathcal{T}_k^+$ is the set of elements of $\mathcal{T}_k$ that are not refined and $\mathcal{T}_k^0$ consists of those elements of $\mathcal{T}_k$ which will eventually be refined. Set

$$\Omega_k^+ = \bigcup_{T\in\mathcal{T}_k^+} \omega_k(T) \quad \text{and} \quad \Omega_k^0 = \bigcup_{T\in\mathcal{T}_k^0} \omega_k(T).$$

Note that the mesh size function $h_k \equiv h_k(x)$ associated with $\mathcal{T}_k$ is monotonically nonincreasing and bounded from below by 0, we have that

$$h_\infty(x) = \lim_{k\to\infty} h_k(x),$$

is well-defined for almost all $x\in\Omega$ and hence defines a function in $L^\infty(\Omega)$. Moreover, the convergence is uniform [35].

Lemma 4.1. *If $\{h_k\}_{k\in\mathbb{N}}$ is the sequence of mesh size functions generated by Algorithm* 4.1*, then*

$$\lim_{k\to\infty}\|h_k-h_\infty\|_{0,\infty,\Omega}=0 \quad \textit{and} \quad \lim_{k\to\infty}\|h_k\chi_{\Omega_k^0}\|_{0,\infty,\Omega}=0,$$

where $\chi_{\Omega_k^0}$ is the characteristic function of Ω_k^0.

Lemma 4.2. *If $\{u_k\}_{k\in\mathbb{N}}$ is the sequence of ground state solutions chosen in Algorithm* 4.1*, then*

$$\lim_{k\to\infty}\max_{T\in\mathcal{M}_k}\eta_k(u_k,T)=0.$$

Proof. We see from the proof of Theorem 4.1 that for any subsequence $\{u_{k_m}\}$ of $\{u_k\}$, there exist a convergent subsequence $\{u_{k_{m_j}}\}$ and $u_\infty\in\mathcal{U}_\infty$ such that

$$u_{k_{m_j}}\to u_\infty, \quad \text{in } H_0^1(\Omega).$$

Now it is sufficient for us to prove that

$$\lim_{j\to\infty}\max_{T\in\mathcal{M}_{k_{m_j}}}\eta_{k_{m_j}}(u_{k_{m_j}},T)=0.$$

In order not to clutter the notation, we shall denote by $\{u_k\}_{k\in\mathbb{N}}$ the subsequence $\{u_{k_{m_j}}\}_{j\in\mathbb{N}}$, and by $\{\mathcal{T}_k\}_{k\in\mathbb{N}}$ the sequence $\{\mathcal{T}_{k_{m_j}}\}_{m\in\mathbb{N}}$.

Let $T_k\in\mathcal{M}_k$ be such that

$$\eta_k(u_k,T_k)=\max_{T\in\mathcal{M}_k}\eta_k(u_k,T).$$

Using Proposition 3.1, we obtain

$$\begin{aligned}\eta_k(u_k,T_k)&\lesssim\|u_k\|_{0,6,\omega_k(T_k)}+\|u_k\|_{1,\omega_k(T_k)}\\&\lesssim\|u_k-u_\infty\|_{1,\Omega}+\|u_\infty\|_{0,6,\omega_k(T_k)}+\|u_\infty\|_{1,\omega_k(T_k)}.\end{aligned}\tag{4.8}$$

Since $T_k\in\mathcal{M}_k\subset\mathcal{T}_k^0$, we have

$$|\omega_k(T_k)|\lesssim h_{T_k}^3\le\|h_k\chi_{\Omega_k^0}\|_{0,\infty,\Omega}^3\to 0, \quad \text{as } k\to\infty,$$

where Lemma 4.1 is used. From Theorem 4.1, we have that the first term in the right hand side of (4.8) tends to zero, too. This completes the proof. ☐

Lemma 4.3. *If $\{u_k\}_{k\in\mathbb{N}}$ is the sequence of ground state solutions chosen in Algorithm* 4.1*, then*

$$\lim_{k\to\infty}\langle\mathbf{R}_k(u_k),v\rangle=0, \quad \forall v\in H_0^1(\Omega).$$

Proof. Using similar arguments as that in the proof of Theorem 4.1, for any subsequence $\{u_{k_m}\}$ of $\{u_k\}$, there exist a convergence subsequence $\{u_{k_{m_j}}\}$ and $u_\infty \in \mathcal{U}_\infty$ such that

$$u_{k_{m_j}} \to u_\infty, \quad \text{in } H_0^1(\Omega),$$

and we need only to prove

$$\lim_{j\to\infty} \langle \mathbf{R}_{k_{m_j}}(u_{k_{m_j}}), v\rangle = 0, \quad \forall v \in H_0^1(\Omega).$$

Since $H_0^2(\Omega)$ is dense in $H_0^1(\Omega)$, it is sufficient to prove

$$\lim_{j\to\infty} \langle \mathbf{R}_{k_{m_j}}(u_{k_{m_j}}), v\rangle = 0, \quad \forall v \in H_0^2(\Omega). \tag{4.9}$$

For simplicity of notation, we denote by $\{u_k\}_{k\in\mathbb{N}}$ the subsequence $\{u_{k_{m_j}}\}_{j\in\mathbb{N}}$, and by $\{\mathcal{T}_k\}_{k\in\mathbb{N}}$ the sequence $\{\mathcal{T}_{k_{m_j}}\}_{j\in\mathbb{N}}$.

Let $v_k \in \mathcal{V}_k$ be the Lagrange's interpolation of v. Since

$$\langle \mathbf{R}_k(u_k), v_k\rangle = 0,$$

we have from Theorem 3.2 that

$$|\langle \mathbf{R}_k(u_k), v\rangle| = |\langle \mathbf{R}_k(u_k), v - v_k\rangle| \le \sum_{T\in\mathcal{T}_k} \eta_k(u_k, T)\|v - v_k\|_{1,\omega_k(T)}.$$

Let $n\in\mathbb{N}$ and $k>n$. By definition, $\mathcal{T}_n^+ \subset \mathcal{T}_k^+ \subset \mathcal{T}_k$. Thus we have

$$\begin{aligned}|\langle \mathbf{R}_k(u_k), v\rangle| \le& \sum_{T\in\mathcal{T}_n^+} \eta_k(u_k, T)\|v - v_k\|_{1,\omega_k(T)} + \sum_{T\in\mathcal{T}_k\setminus\mathcal{T}_n^+} \eta_k(u_k, T)\|v - v_k\|_{1,\omega_k(T)} \\ \le& \eta_k(u_k, \mathcal{T}_n^+)\|v - v_k\|_{1,\Omega_n^+(T)} + \eta_k(u_k, \mathcal{T}_k \setminus \mathcal{T}_n^+)\|v - v_k\|_{1,\Omega_n^0(T)}.\end{aligned}$$

Using Proposition 3.1, we get

$$\eta_k(u_k, \mathcal{T}_k \setminus \mathcal{T}_n^+) \le \eta_k(u_k, \mathcal{T}_k) \le C_\eta,$$

which together with the interpolation estimate yields

$$|\langle \mathbf{R}_k(u_k), v\rangle| \lesssim (\eta_k(u_k, \mathcal{T}_n^+) + C_\eta \|h_n \chi_{\Omega_n^0}\|_{0,\infty,\Omega})\|v\|_{2,\Omega}. \tag{4.10}$$

Now we shall use (4.10) to prove (4.9). Let $\varepsilon>0$ be arbitrary, Lemma 4.1 implies that there exists $n\in\mathbb{N}$, such that

$$C_\eta \|h_n \chi_{\Omega_n^0}\|_{0,\infty,\Omega} < \varepsilon. \tag{4.11}$$

Since $\mathcal{T}_n^+ \subset \mathcal{T}_k^+ \subset \mathcal{T}_k$ and the marking strategy (4.1) is reasonable, we arrive at

$$\eta_k(u_k, \mathcal{T}_n^+) \leq (\#\mathcal{T}_n^+)^{\frac{1}{2}} \max_{T\in\mathcal{T}_n^+} \eta_k(u_k, T) \leq (\#\mathcal{T}_n^+)^{\frac{1}{2}} \max_{T\in\mathcal{M}_k} \eta_k(u_k, T).$$

By Lemma 4.2, we can select $N \geq n$ such that

$$\eta_k(u_k, \mathcal{T}_n^+) < \varepsilon, \quad \forall k > N. \tag{4.12}$$

So, we obtain (4.9) by combining (4.10), (4.11) and (4.12). This completes the proof. □

Finally, we prove the main result of this paper.

Theorem 4.2. *Given a sufficiently fine initial mesh $\mathcal{T}_0$. If $\{\mathcal{U}_k\}_{k\in\mathbb{N}}$ is the sequence of adaptive finite element approximations generated by Algorithm* 4.1, *then*

$$\lim_{k\to\infty} E_k = \min_{v\in\mathcal{A}} E(v), \tag{4.13a}$$

$$\lim_{k\to\infty} \mathrm{dist}_{H^1}(\mathcal{U}_k, \mathcal{U}) = 0, \tag{4.13b}$$

$$\lim_{k\to\infty} \mathrm{dist}(\Lambda_k, \Lambda) = 0. \tag{4.13c}$$

Proof. Let $u_k \in \mathcal{U}_k$ be the sequence of ground state solutions chosen in Algorithm 4.1, and (λ_k, u_k) solve (3.3) for $k=1,2,\cdots$. It is known from Theorem 4.1 that for any subsequence $\{u_{k_m}\}$ of $\{u_k\}$, there exist a convergent subsequence $\{u_{k_{m_j}}\}$ and $u_\infty \in \mathcal{U}_\infty$ such that

$$u_{k_{m_j}} \to u_\infty, \quad \text{in } H_0^1(\Omega) \quad \text{and} \quad \lambda_{k_{m_j}} \to \lambda_\infty,$$

where $(\lambda_\infty, u_\infty)$ solves (3.3). It is sufficient for us to prove that $u_\infty \in \mathcal{U}$, which leads to (4.13a) and (4.13b) directly, and implies (4.13c) by noting (2.1) and (3.3). For simplicity, we denote by $\{u_k\}_{k\in\mathbb{N}}$ the convergent subsequence $\{u_{k_{m_j}}\}_{j\in\mathbb{N}}$, and by $\{\mathcal{T}_k\}_{k\in\mathbb{N}}$ the subsequence $\{\mathcal{T}_{k_{m_j}}\}_{j\in\mathbb{N}}$.

We first prove that limiting eigenpair $(\lambda_\infty, u_\infty)$ is also an eigenpair of (2.1). Note that

$$\begin{aligned}
&\lambda_\infty(u_\infty, v) - \alpha(\nabla u_\infty, \nabla v) - (Vu_\infty + \mathcal{N}(u_\infty^2)u_\infty, v) - \langle \mathbf{R}_k(u_k), v\rangle \\
=&(\lambda_\infty u_\infty - \lambda_k u_k, v) - \alpha(\nabla(u_\infty - u_k), \nabla v) \\
&- (V(u_\infty - u_k), v) - (\mathcal{N}(u_\infty^2)u_\infty - \mathcal{N}(u_k^2)u_k, v), \quad \forall v \in H_0^1(\Omega),
\end{aligned}$$

we obtain from (2.6) that

$$\begin{aligned}
&|\lambda_\infty(u_\infty, v) - \alpha(\nabla u_\infty, \nabla v) - (Vu_\infty + \mathcal{N}(u_\infty^2)u_\infty, v) - \langle \mathbf{R}_k(u_k), v\rangle| \\
\lesssim&\|\nabla(u_\infty - u_k)\|_{0,\Omega}\|\nabla v\|_{0,\Omega} + \|V\|_{0,\Omega}\|u_\infty - u_k\|_{0,3,\Omega}\|v\|_{0,6,\Omega} \\
&+ \|u_\infty - u_k\|_{1,\Omega}\|v\|_{1,\Omega} + (\|u_\infty - u_k\|_{0,\Omega} + |\lambda_k - \lambda_\infty|)\|v\|_{0,\Omega}, \quad \forall v \in H_0^1(\Omega).
\end{aligned} \tag{4.14}$$

Since $\lambda_k \to \lambda_\infty$ and $u_k \to u_\infty$ in $H_0^1(\Omega)$, the right hand side of (4.14) tends to zero when k tends to infinity. Using Lemma 4.3 and identity

$$\begin{aligned}&\lambda_\infty(u_\infty, v) - \alpha(\nabla u_\infty, \nabla v) - (Vu_\infty + \mathcal{N}(u_\infty^2)u_\infty, v)\\ =&\lambda_\infty(u_\infty, v) - \alpha(\nabla u_\infty, \nabla v) - (Vu_\infty + \mathcal{N}(u_\infty^2)u_\infty, v) - \langle \mathbf{R}_k(u_k), v\rangle + \langle \mathbf{R}_k(u_k), v\rangle,\end{aligned}$$

we arrive at

$$\alpha(\nabla u_\infty, \nabla v) + (Vu_\infty + \mathcal{N}(u_\infty^2)u_\infty, v) = \lambda_\infty(u_\infty, v), \quad \forall v \in H_0^1(\Omega).$$

Now we prove that for a sufficiently fine initial mesh, the limiting eigenfunction u_∞ is a ground state solution. Set

$$\mathcal{W} = \big\{w \in H_0^1(\Omega) : w \text{ is an eigenfunction of (2.1)}\big\}.$$

Note that $\mathcal{U} \subsetneq \mathcal{W}$, the ground state solutions in $\mathcal{U}$ minimize energy functional (2.2), which is continuous over $H_0^1(\Omega)$, we can choose a mesh $\mathcal{T}_0$ such that

$$E_0 \equiv E(v) < \min_{w \in \mathcal{W} \backslash \mathcal{U}} E(w), \quad \forall v \in \mathcal{U}_0,$$

where the fact

$$\lim_{h \to 0} \inf_{v \in S_0^h(\Omega)} \|v - w\|_{1,\Omega} = 0, \quad \forall w \in H_0^1(\Omega),$$

is used. Due to $\mathcal{T}_k \subset \mathcal{T}_0$, we have $E_k \le E_0$ and obtain $u_\infty \in \mathcal{U}$. This completes the proof. □

If we make a further assumption that

$$\mathcal{F}''(t) > 0, \quad \text{for } \ t \in [0, \infty), \tag{4.15}$$

then energy functional

$$E(\sqrt{\rho}) = \int_\Omega \big(\alpha|\nabla\sqrt{\rho}|^2 + V(x)\rho(x) + \mathcal{F}(\rho(x))\big)dx + \frac{1}{2q}D_K(\rho^q, \rho^q),$$

is strictly convex on convex set $\{\rho \ge 0 : \sqrt{\rho} \in \mathcal{A}\}$ and hence there exists a unique minimizer of (2.2) in admissible class $\mathcal{A}$. Note that the minimizer of (2.2) in V_k is unique when initial mesh $\mathcal{T}_0$ is fine enough (c.f., e.g., [43]), we have

Corollary 4.1. Assume that the hypothesis of Theorem 4.2 and (4.15) are satisfied. If $(\lambda, u) \in \mathbb{R} \times \mathcal{A}$ is the ground state solution of (2.1) and $(\lambda_k, u_k) \in \mathbb{R} \times V_k$ is the ground state solution of (3.3), then

$$\lim_{k \to \infty} \|u_k - u\|_{1,\Omega} = 0, \qquad \lim_{k \to \infty} |\lambda_k - \lambda| = 0.$$

5 Numerical examples

In this section, we will report on some numerical experiments for both linear finite elements and quadratic finite elements in three dimensions to illustrate the convergence of adaptive finite element approximations of energy.

Our numerical computations are carried out on LSSC-II in the State Key Laboratory of Scientific and Engineering Computing, Chinese Academy of Sciences, and our codes are based on the toolbox PHG of the laboratory. The ground state solutions are obtained by directly minimizing the energy functional (2.2) using conjugate gradient method. All of the computational results are given in atomic unit (a.u.).

Example 5.1. Consider the ground state solution of GPE for BEC with a harmonic oscillator potential

$$V(x,y,z)=\frac{1}{2}(\gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2),$$

where γ_x=1, γ_y=2, γ_z=4. We solve the following nonlinear problem: find $(\lambda,u)\in\mathbb{R}\times H_0^1(\Omega)$, such that $\|u\|_{0,\Omega}$=1 and

$$\begin{cases} \Big(-\dfrac{1}{2}\Delta+V+\beta|u|^2\Big)u=\lambda u, & \text{in } \Omega,\\ u=0, & \text{on } \partial\Omega,\end{cases}$$

where β=200 and $\Omega=[-8,8]\times[-6,6]\times[-4,4]$.

The convergence of energies and the reduction of the a posteriori error estimators are presented in Fig. 1, which support our theory and proof. Some cross-sections of the adaptively refined meshes constructed by the a posteriori error indicators are displayed in Fig. 2.

In the next two examples, we shall carry out the ground state energy calculations of atomic and molecular systems based on TFW type orbital-free models. The nonlinear term is given by

$$\mathcal{N}(u^2)=\int_\Omega\frac{u^2(y)}{|\cdot-y|}dy+\frac{5}{3}C_{TF}u^{\frac{4}{3}}+v_{xc}(u^2),$$

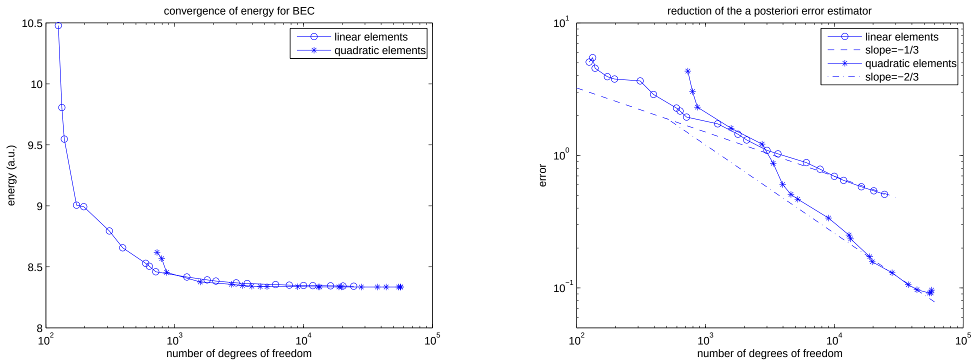
where $C_{TF}=3(3\pi^2)^{2/3}/10$ and v_{xc} is the exchange-correction potential. The exchange-correction potential used in our computation is chosen as

$$v_{xc}(\rho)=v_x^{LDA}(\rho)+v_c^{LDA}(\rho), \tag{5.1}$$

where

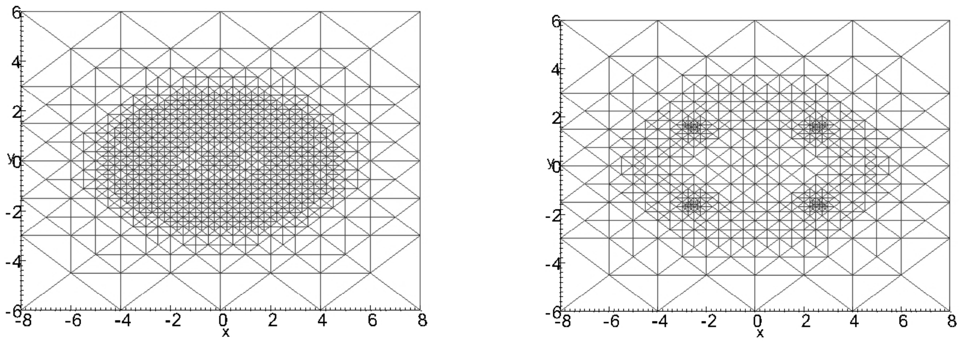
$$v_x^{LDA}(\rho)=-\Big(\frac{3}{\pi}\Big)^{\frac{1}{3}}\rho^{\frac{1}{3}},$$

$$v_c^{LDA}(\rho)=\begin{cases} 0.0311\ln r_s-0.0584+0.0013r_s\ln r_s-0.0084r_s, & \text{if } r_s<1,\\ -\dfrac{0.1423+0.0633r_s+0.1748\sqrt{r_s}^2}{(1+1.0529\sqrt{r_s}+0.3334r_s)}, & \text{if } r_s\geq 1,\end{cases}$$



(a) (b)

Figure 1: (a): Convergence curves of energy for BEC. (b): Reduction of the a posteriori error estimators using linear and quadratic elements.



(a) (b)

Figure 2: The cross-sections on $z = 0$ of adaptive meshes using linear (a) and quadratic (b) elements.

and

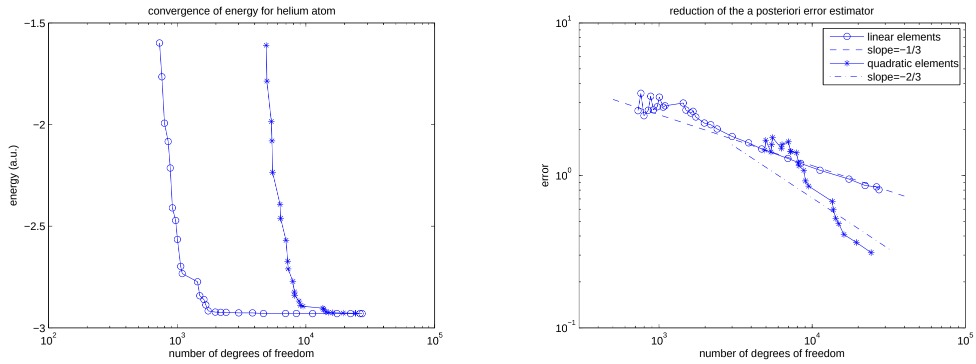
$$r_s = \left(\frac{3}{4\pi\rho}\right)^{\frac{1}{3}}.$$

Example 5.2. Consider the TFW type orbital-free model for helium atoms. The external electrostatic potential is

$$V(x) = -\frac{2}{|x|}.$$

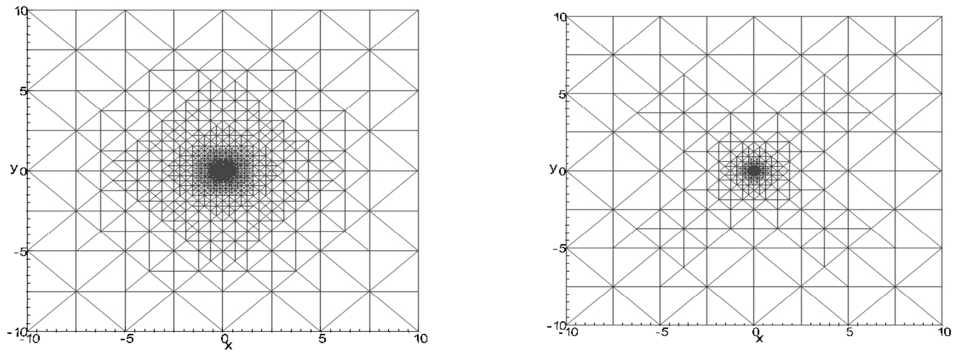
Then we have the following nonlinear problem: find $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$ such that $\|u\|_{0,\Omega}^2 = 2$ and

$$\begin{cases} -\dfrac{1}{10}\Delta u - \dfrac{2}{|x|}u + u\displaystyle\int_\Omega \frac{|u(y)|^2}{|x-y|}dy + \frac{5}{3}C_{TF}u^{\frac{7}{3}} + v_{xc}(u^2)u = \lambda u, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, \end{cases}$$



(a) (b)

Figure 3: (a): Convergence curves of energy for the helium atom. (b): Reduction of the a posteriori error estimators using linear and quadratic elements.



(a) (b)

Figure 4: The cross-sections on $z=0$ of adaptive meshes using linear (a) and quadratic (b) elements.

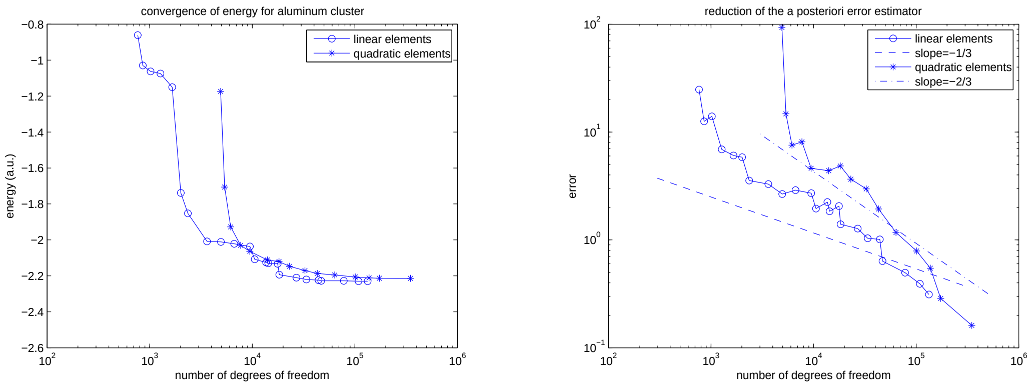
where $\Omega=(-5.0,5.0)^3$.

The convergence of energies and the reduction of the a posteriori error estimators are shown in Fig. 3, which support our theory. The cross-sections of the adaptive meshes are displayed in Fig. 4, from which we observe that more refined meshes (nodes) appear in the area where the nuclei are located.

Example 5.3. Finally, we consider an aluminum cluster in the face centered cubic lattice consisting of $3\times 3\times 3$ unit cells with 172 aluminium atoms, where the GHN pseudopotential [25] is used. We solve the following nonlinear problem: find $(\lambda,u)\in\mathbb{R}\times H_0^1(\Omega)$ such that $\|u\|_{0,\Omega}^2=172$ and

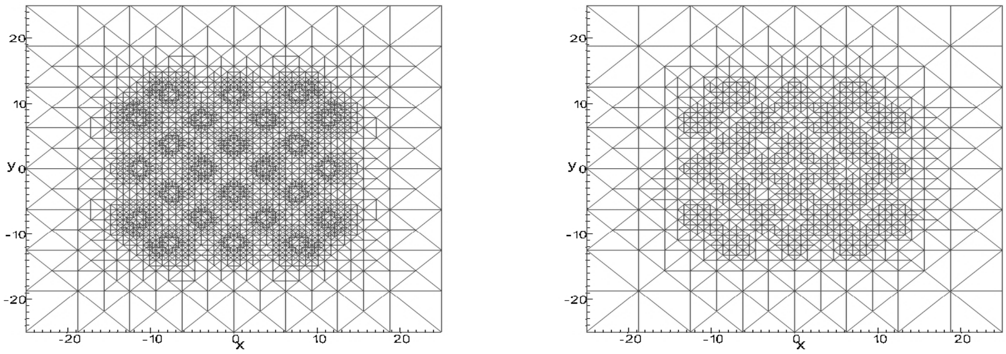
$$\begin{cases} -\dfrac{1}{10}\Delta u+V_{pseu}^{GHN}u+u\displaystyle\int_\Omega\frac{|u(y)|^2}{|x-y|}dy+\frac{5}{3}C_{TF}u^{\frac{7}{3}}+v_{xc}(u^2)u=\lambda u, & \text{in } \Omega,\\ u=0, & \text{on } \partial\Omega, \end{cases}$$

where $\Omega=(-25.0,25.0)^3$.



(a) (b)

Figure 5: (a): Convergence curves of energy for the aluminium cluster in FCC lattice. (b): Reduction of the a posteriori error estimators using linear and quadratic elements.



(a) (b)

Figure 6: The cross-sections on $z = 0$ of adaptive meshes using linear (a) and quadratic (b) finite elements.

The convergence of energies and the reduction of a posteriori error estimators are shown in Fig. 5. The cross-sections of the adaptive meshes are displayed in Fig. 6. We observe that with the a posteriori error estimators, the refinement is carried out automatically at the regions where the computed functions vary rapidly, especially near the nuclei. As a result, the computational accuracy can be controlled efficiently and the computational cost is reduced significantly.

6 Conclusions

We have analyzed adaptive finite element approximations for ground state solutions of a class of nonlinear eigenvalue problems. We have proved that the adaptive finite element loop produces a sequence of approximations that converge to the set of exact ground state solutions. This result covers many mathematical models of practical interest, for instance, the Bose-Einstein condensation, the TFW model in the orbital-free density functional theory, and Schrödinger-Newton equations in the quantum state reduction [13, 26, 36] where the integration kernel K is negative. We have also applied adaptive finite element discretizations to micro-structure of matter calculations, which support our theory. It is shown by Fig. 1, Fig. 3, and Fig. 5 that we may have some convergence rates of adaptive finite element approximations of energy. We refer to [14] for the study of convergence rate and optimal complexity of adaptive finite element approximations for a class of nonlinear eigenvalue problems, which requires some new technical tools.

Appendix

We may follow the framework in [40] to derive an upper bound and a lower bound of the a posteriori error estimate. Let

$$\begin{aligned}&X = Y = H_0^1(\Omega), \qquad \|\cdot\|_X = \|\cdot\|_Y = \|\cdot\|_{1,\Omega},\\&\langle F(\lambda,u),(\mu,v)\rangle = \int_\Omega \big(\alpha\nabla u\nabla v + Vuv + \mathcal{N}(u^2)uv - \lambda uv\big) + \mu\Big(\int_\Omega u^2 - Z\Big).\end{aligned}$$

It is seen that (2.1) may be written as

$$F(\lambda,u) = 0, \tag{A.1}$$

and $F\in C^1(\mathbb{R}\times X, \mathbb{R}\times Y^*)$, where Y^* is the dual space of Y. A solution (λ,u) of (A.1) is said to be regular if the following equation

$$DF(\lambda,u)\cdot(\mu,v) = (\kappa,f),$$

is uniquely solvable in $\mathbb{R}\times X$ for each $(\kappa,f)\in\mathbb{R}\times Y^*$, where

$$DF(\lambda,u): \mathbb{R}\times X \to \mathbb{R}\times Y^*,$$

is the Fréchet derivative of F at (λ,u). It is seen that $(\lambda,u)\in\mathbb{R}\times H_0^1(\Omega)$ is a regular solution of (A.1) if

$$\langle (E''(u)-\lambda)v, v\rangle_{Y^*,X} \geq \gamma\|\nabla v\|_{0,\Omega}^2, \quad \forall v\in H_0^1(\Omega)\cap u^\perp, \tag{A.2}$$

is true for some constant $\gamma>0$ (c.f., e.g., [29]), where

$$\begin{aligned}\langle (E''(u)-\lambda)v,w\rangle = {} & \alpha(\nabla v,\nabla w) + ((V+\mathcal{N}(u^2)-\lambda)v,w) + 2(\mathcal{N}_1'(u^2)u^2v,w)\\&+ 2qD_K(u^{2q-1}v,u^{2q-1}w) + 2(q-1)(\mathcal{N}_2(u^2)v,w),\end{aligned}$$

and

$$u^\perp = \big\{w\in L^2(\Omega): (u,w)=0\big\}.$$

It has been proved that (A.2) is satisfied by some special TFW models that are of convex functional (see, e.g., [9, 10]).

Let

$$X_h = Y_h = S_0^h(\Omega),$$

and define

$$\langle F_h(\lambda_h, u_h), (\mu, v)\rangle = \langle F(\lambda_h, u_h), (\mu, v)\rangle, \quad \forall (\mu, v) \in \mathbb{R} \times S_0^h(\Omega).$$

We see that $F_h \in C(\mathbb{R} \times X_h, \mathbb{R} \times Y_h^*)$ and is an approximation of F. Obviously, finite element eigenvalue problem (3.3) is equivalent to

$$F_h(\lambda_h, u_h) = 0,$$

and (λ_h, u_h) is an approximate solution of (A.1).

The following proposition in [40, Section 2.1] yields a posteriori error estimates in the neighborhood of (λ, u) that satisfies (A.1).

Proposition 6.1. *Let (λ, u) be a regular solution of* (A.1)*. If DF is the derivative of F and DF is Lipschitz continuous at (λ, u), then the following estimate holds for all (λ_h, u_h) sufficiently close to this solution:*

$$\|F(\lambda_h, u_h)\|_{\mathbb{R}\times Y^*} \lesssim |\lambda_h - \lambda| + \|u_h - u\|_X \lesssim \|F(\lambda_h, u_h)\|_{\mathbb{R}\times Y^*}. \tag{A.3}$$

It is shown from (A.3) that $\|F(\lambda_h, u_h)\|_{\mathbb{R}\times Y^*}$ is a posteriori error estimator. When we apply the general approach in [40, Sections 3.3-3.4] to

$$\underline{a}(x, u, \nabla u) = \alpha \nabla u \quad \text{and} \quad b(x, u, \nabla u) = \lambda u - V u - \mathcal{N}(u^2) u,$$

by taking

$$\begin{aligned} &\underline{a}_h(x, u_h, \nabla u_h) = \alpha \nabla u_h, && b_h(x, u_h, \nabla u_h) = \overline{\lambda u_h} - \overline{V u_h} - \overline{\mathcal{N}(u_h^2) u_h}, \\ &\eta_T = \eta_h(u_h, T), && \varepsilon_T = \mathrm{osc}_h(u_h, T), \end{aligned}$$

we then give a proof of Theorem 3.1.

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