

EIGENFUNCTION BEHAVIOR AND ADAPTIVE FINITE ELEMENT APPROXIMATIONS OF NONLINEAR EIGENVALUE PROBLEMS IN QUANTUM PHYSICS

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Abstract. In this paper, we investigate a class of nonlinear eigenvalue problems resulting from quantum physics. We first prove that for any open set G , there exists an eigenfunction that cannot be a polynomial on G , which may be reviewed as a refinement of the classic unique continuation property. Then we apply the non-polynomial behavior of the eigenfunction to show that the adaptive finite element approximations are convergent even if the initial mesh is not fine enough. We finally remark that similar arguments can be applied to a class of linear eigenvalue problems that improve the relevant existing results.

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1. INTRODUCTION

In this paper, we investigate the eigenfunction behavior and adaptive finite element approximations of the following nonlinear eigenvalue problem: find $(\lambda_i, \phi_i) \in \mathbb{R} \times H_0^1(\Omega)$ such that $\int_{\Omega} \phi_i \phi_j = \delta_{ij}$ ($i, j = 1, 2, \dots, N$) and

$$(-\kappa\Delta + V + \mathcal{N}(\rho))\phi_i = \lambda_i\phi_i, \quad \text{in } \Omega, \quad i = 1, 2, \dots, N, \quad (1.1)$$

where $\Omega \subset \mathbb{R}^3$, $N \geq 1$, $\kappa > 0$, $\rho = \sum_{i=1}^N |\phi_i|^2$, $V : \Omega \rightarrow \mathbb{R}$ is a given function, and \mathcal{N} maps a nonnegative function to some function on Ω . We observe that the Schrödinger–Newton equation modeling the quantum state reduction [18, 25], the Gross–Pitaevskii equation (GPE) describing Bose–Einstein condensates (BEC) [2, 35], and the Thomas–Fermi–von Weizsäcker (TFvW) type equations and the Kohn–Sham equations appearing in the electronic density functional theory [3, 9, 20–22] are typical examples of (1.1).

We understand that it is significant to solve (1.1) accurately and efficiently. And we note that the *a priori* knowledge of their eigenfunctions is very helpful in the design and analysis of numerical methods. To improve the approximation accuracy and reduce the computational cost in solving the eigenvalue problem, we see from the regularity behavior of eigenfunctions [17, 34] that adaptive finite element approaches should be employed

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(see also [7, 10–14, 24, 31] and references cited therein). We observe that the adaptive finite element analysis of the nonlinear eigenvalue problem (1.1) in [7, 8, 10] requires that the initial mesh size is small enough. However, our numerical experiments show that the small initial mesh size requirement is unnecessary [7, 8, 10]. In this paper, we study the adaptive finite element approximations when the initial mesh is not fine, for which we need to apply an eigenfunction behavior that is also investigated.

We see that the unique continuation property is significant in the context of partial differential equations (see, *e.g.*, [19, 28, 33] and references cited therein). After looking into the eigenfunction behavior of (1.1), we find that for any open set G , there exists an eigenfunction that cannot be a polynomial on G , which may be reviewed as a refinement of the classic unique continuation property and is indeed a key in our adaptive finite element analysis. Taking into account the eigenfunction behavior, we are indeed able to prove the convergence of adaptive finite element approximations without the requirement of the small initial mesh size.

The rest of this paper is organized as follows. In the next section, we describe some basic notation and review the adaptive finite element method for solving (1.1). Then we show some polynomial properties which are crucial in our adaptive finite element analysis. In Section 3, we obtain that for any open set G of Ω , there exists an eigenfunction of (1.1) that cannot be a polynomial on G under some assumptions, which may be reviewed as an extension and refinement of the classic unique continuation property. In Section 4, based on the non-polynomial behavior of eigenfunctions, we study the convergence of the adaptive finite element method. We finally remark that similar arguments can be applied to a class of linear eigenvalue problems that improve the relevant existing results.

2. PRELIMINARIES

Let $\Omega \subset \mathbb{R}^3$ be a convex polyhedral bounded domain. We will always use G for a nonempty open set of \mathbb{R}^d ($d \geq 1$) throughout this paper. Let $\mathbb{Q}_+ = \mathbb{Q} \cap [0, \infty)$ and $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_d) \in \mathbb{Q}_+^d$ be a d -tuple. We denote $|\alpha| = \alpha_1 + \alpha_2 + \dots + \alpha_d$, define $x^\alpha = \xi_1^{\alpha_1} \xi_2^{\alpha_2} \xi_3^{\alpha_3}$ for any $x = (\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3$ and $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{Q}_+^3$, and use the notation

$$\partial_i \phi = \frac{\partial \phi}{\partial \xi_i}, \quad i = 1, 2, 3.$$

For any $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_d), \beta = (\beta_1, \beta_2, \dots, \beta_d) \in \mathbb{Q}_+^d$, we denote $\alpha \succ \beta$ if the first non-zero element of $\alpha - \beta = (\alpha_1 - \beta_1, \alpha_2 - \beta_2, \dots, \alpha_d - \beta_d)$ is larger than 0 and $\alpha \succcurlyeq \beta$ if $\alpha \succ \beta$ or $\alpha = \beta$. For convenience, we define

$$\mathcal{P}_{\mathbb{Q}_+}(G) = \left\{ \sum_{\alpha \in I \subset \mathbb{Q}_+^d} a_\alpha x^\alpha : a_\alpha, x^\alpha \in \mathbb{R}, \forall \alpha \in I, \forall x \in G, |I| < \infty \right\},$$

where $|I|$ means the cardinality of I . We shall use the notation

$$\mathcal{P}_{\mathbb{Q}_+}^\mu(G) = \{p^\mu : p \in \mathcal{P}_{\mathbb{Q}_+}(G) \text{ and } p^\mu(x) \in \mathbb{R} \forall x \in G\}$$

for any $\mu \geq 0$. We call $a_\alpha x^\alpha$ with $a_\alpha \neq 0$ a monomial. Denote $|\alpha|$ the degree of the monomial $a_\alpha x^\alpha$. We shall let the degree of the polynomial 0 be $-\infty$. For any $p \in \mathcal{P}_{\mathbb{Q}_+}(G)$, define $\deg p$ as the max degree of terms of p , which is called the degree of p . We shall also denote $\deg p^\mu = \mu \deg p$ for any $p \in \mathcal{P}_{\mathbb{Q}_+}(G)$ and $\mu \in \mathbb{Q}_+$ and $\deg(p/q) = \deg p - \deg q$ for any $p, q \in \mathcal{P}_{\mathbb{Q}_+}(G)$. Let $\mathcal{P}_\ell(G)$ be the set of real polynomials on G with a degree not larger than ℓ . It is clear that $\mathcal{P}_\ell(G) \subset \mathcal{P}_{\mathbb{Q}_+}(G)$. The standard notation $W^{s,p}(\Omega)$ ($s \geq 0$) for Sobolev spaces and their associated norms $\|\cdot\|_{s,p,\Omega}$ shall also be used [1]. We write

$$G \subset\subset \Omega$$

if $\bar{G} \subset \Omega$ and \bar{G} is compact. $W_{\text{loc}}^{s,p}(\Omega)$ denotes the space of the function v satisfying that for any open set $G \subset\subset \Omega$, $v \in W^{s,p}(G)$. For $p = 2$, we denote $H^s(\Omega) = W^{s,2}(\Omega)$, $H_{\text{loc}}^s(\Omega) = W_{\text{loc}}^{s,2}(\Omega)$, $H_0^1(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\}$,

where $v|_{\partial\Omega}$ is understood in the sense of trace, $\|\cdot\|_{s,\Omega} = \|\cdot\|_{s,2,\Omega}$. We use $\mathcal{P}(s, (c_1, c_2))$ to denote a class of functions satisfying some growth conditions:

$$\mathcal{P}(s, (c_1, c_2)) = \{f : \exists a_1, a_2 \in \mathbb{R} \text{ such that } c_1 t^s + a_1 \leq f(t) \leq c_2 t^s + a_2 \quad \forall t \geq 0\}$$

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

2.1. Quantum eigenvalue problem

We consider the nonlinear eigenvalue problem (1.1) where V is of the form

$$V = - \sum_{j=1}^M \frac{f_j}{g_j} \quad (2.1)$$

with $f_j, g_j \in \mathcal{P}_{\mathbb{Q}_+}^\mu(\mathbb{R}^3)$ ($j = 1, 2, \dots, M$) for some $\mu \in \mathbb{Q}_+$. Assume that \mathcal{N} is divided into two parts:

$$\mathcal{N}(\rho) = \mathcal{N}_1(\rho) + \mathcal{N}_2(\rho), \quad (2.2)$$

where $\rho = \sum_{i=1}^N |\phi_i|^2$. Let $\mathcal{N}_1 : [0, \infty) \rightarrow \mathbb{R}$ be defined by

$$\mathcal{N}_1(t) = \sum_{i=1}^K \frac{p_i(t)}{h_i(t)} \ln q_i(t) \quad (2.3)$$

with $p_i, h_i \in \mathcal{P}_{\mathbb{Q}_+}([0, \infty))$, where q_i are polynomials satisfying $q_i|_{[0, \infty)} > 0$ and $q_i \neq 1$ ($i = 1, 2, \dots, K$), and \mathcal{N}_2 be given by a convolution integral

$$\mathcal{N}_2(\rho) = \alpha \int_{\Omega} \frac{\rho(y)}{|\cdot - y|} dy \quad (2.4)$$

with some constant α .

The energy functional associated with (1.1) is

$$E(\Phi) = \int_{\Omega} \left(\kappa \sum_{i=1}^N |\nabla \phi_i|^2 + V \rho_{\Phi} + \mathcal{E}(\rho_{\Phi}) \right) + \frac{\alpha}{2} D(\rho_{\Phi}, \rho_{\Phi})$$

for $\Phi = (\phi_1, \phi_2, \dots, \phi_N) \in \mathcal{H} \equiv (H_0^1(\Omega))^N$, where $\rho_{\Phi} = \sum_{i=1}^N |\phi_i|^2$, $\mathcal{E} : [0, \infty) \rightarrow \mathbb{R}$ is defined by

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

and $D(\cdot, \cdot)$ is a bilinear form as follows

$$D(f, g) = \int_{\Omega} \int_{\Omega} \frac{f(x)g(y)}{|x - y|} dx dy.$$

For any $\Phi \in \mathcal{H}$, we denote

$$\|\Phi\|_{s,\Omega} = \left(\sum_{i=1}^N \|\phi_i\|_{s,\Omega}^2 \right)^{1/2}.$$

We see that (1.1) includes the GPE, the Schrödinger–Newton equation, the TFvW type equation, and the Kohn–Sham equation (see Rem. 3.7, Examples 3.9, 3.10, and 3.11 for more details).

Let \mathcal{Q} be a subset of \mathcal{H} :

$$\mathcal{Q} = \{\Phi \in \mathcal{H} : \Phi^T \Phi = I^{N \times N}\},$$

where $\Phi^T \Psi = \left(\int_{\Omega} \phi_i \psi_j \right) \in \mathbb{R}^{N \times N}$. The ground state charge density of (1.1) is obtained by solving the minimization problem

$$\inf\{E(\Phi) : \Phi \in \mathcal{Q}\}. \quad (2.5)$$

We see that any minimizer $\Phi = (\phi_1, \dots, \phi_N)$ of (2.5) satisfies

$$\begin{cases} \langle H_{\Phi} \phi_i, v \rangle = \left(\sum_{j=1}^N \lambda_{ji} \phi_j, v \right) & \forall v \in H_0^1(\Omega), \quad i = 1, 2, \dots, N, \\ \int_{\Omega} \phi_i \phi_j = \delta_{ij}, \end{cases} \quad (2.6)$$

where $H_{\Phi} : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$ is the Hamiltonian operator defined by

$$\langle H_{\Phi} u, v \rangle = \kappa(\nabla u, \nabla v) + (V \rho_{\Phi} + \mathcal{N}(\rho_{\Phi})u, v) \quad \forall u, v \in H_0^1(\Omega)$$

and

$$\Lambda = (\lambda_{ij})_{i,j=1}^N = \left(\int_{\Omega} \phi_i H_{\Phi} \phi_j \right)_{i,j=1}^N$$

is the Lagrange multiplier. We call (Λ, Φ) a state of (2.6) and define the set of ground states by

$$\Theta = \left\{ (\Lambda, \Phi) \in \mathbb{R}^{N \times N} \times \mathcal{Q} : E(\Phi) = \min_{\Psi \in \mathcal{Q}} E(\Psi) \text{ and } (\Lambda, \Phi) \text{ solves (2.6)} \right\}.$$

We define the set of states of (2.6) by

$$\mathcal{W} = \{(\Lambda, \Phi) \in \mathbb{R}^{N \times N} \times \mathcal{H} : (\Lambda, \Phi) \text{ solves (2.6)}\}.$$

Since the electron density ρ_{Φ} and the operator H_{Φ} are invariant under any unitary transform, we may diagonalize the Lagrange multiplier Λ and arrive at

$$\begin{cases} \langle H_{\Phi} \phi_i, v \rangle = \lambda_i(\phi_i, v) & \forall v \in H_0^1(\Omega), \quad i = 1, 2, \dots, N, \\ \int_{\Omega} \phi_i \phi_j = \delta_{ij}, \end{cases} \quad (2.7)$$

which is equivalent to (2.6) and a weak form of (1.1).

In practice, the ground states are usually approximated by solving the lowest N eigenpairs of (2.7) [22].

2.2. An adaptive finite element method

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

$$\frac{h_{\tau}}{\rho_{\tau}} \leq \gamma^* \quad \forall \tau \in \mathcal{T}_h,$$

where h_{τ} is the diameter of τ , ρ_{τ} is the diameter of the biggest ball contained in τ , and $h = \max\{h_{\tau} : \tau \in \mathcal{T}_h\}$. Let \mathcal{E}_h denote the set of interior faces of \mathcal{T}_h . We shall also use a slight abuse of notation that h denotes the mesh size function defined by

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

Let $S^h(\Omega) \subset H^1(\Omega)$ be the corresponding finite element space consisting of continuous piecewise polynomials over \mathcal{T}_h of degrees not larger than $n \geq 1$ and

$$S_0^h(\Omega) = S^h \cap H_0^1(\Omega).$$

Let $V_h = (S_0^h(\Omega))^N$.

Consider the finite element approximation of (2.5):

$$\inf \{E(\Phi_h) : \Phi_h \in V_h \cap \mathcal{Q}\}. \quad (2.8)$$

We see that any minimizer $\Phi_h = (\phi_{1,h}, \dots, \phi_{N,h})$ of (2.8) solves the Euler-Lagrange equation

$$\begin{cases} \langle H_{\Phi_h} \phi_{i,h}, v \rangle = \left(\sum_{j=1}^N \lambda_{ji,h} \phi_{j,h}, v \right) & \forall v \in S_0^h(\Omega), \quad i = 1, 2, \dots, N, \\ \int_{\Omega} \phi_{i,h} \phi_{j,h} = \delta_{ij} \end{cases} \quad (2.9)$$

with the Lagrange multiplier

$$\Lambda_h = (\lambda_{ij,h})_{i,j=1}^N = \left(\int_{\Omega} \phi_{i,h} H_{\Phi_h} \phi_{j,h} \right)_{i,j=1}^N$$

when the energy functional is differentiable. Define the set of finite dimensional ground state solutions:

$$\Theta_h = \left\{ (\Lambda_h, \Phi_h) \in \mathbb{R}^{N \times N} \times (\mathcal{Q} \cap V_h) : E(\Phi_h) = \min_{\Psi \in \mathcal{Q} \cap V_h} E(\Psi), (\Lambda_h, \Phi_h) \text{ solves (2.9)} \right\}.$$

Using a unitary transformation, we have the following discrete equation

$$\begin{cases} \langle H_{\Phi_h} \phi_{i,h}, v \rangle = \lambda_{i,h}(\phi_{i,h}, v) & \forall v \in H_0^1(\Omega), \quad i = 1, 2, \dots, N, \\ \int_{\Omega} \phi_{i,h} \phi_{j,h} = \delta_{ij}. \end{cases} \quad (2.10)$$

In practice, we usually solve and obtain the lowest N eigenpairs of (2.10) [22].

We recall that the adaptive finite element method is to repeat the following procedure [10]:

Solve \rightarrow Estimate \rightarrow Mark \rightarrow Refine.

For convenience, we shall replace subscript h (or h_k) by an iteration counter k of the adaptive method afterwards.

Given an initial triangulation \mathcal{T}_0 so that the dimension of S_0^h is larger than or equal to N , the above procedure generates a sequence of nested triangulations \mathcal{T}_k ($k = 1, 2, \dots$). Given an iteration counter k , the procedure ‘‘Solve’’ is to get the discrete ground state solution of (2.9) over \mathcal{T}_k . The procedure ‘‘Estimate’’ determines the element indicators for all elements $\tau \in \mathcal{T}_k$. In this step, a posteriori error estimators play a critical role. Then, the element indicators are used by the procedure ‘‘Mark’’ to create a subset \mathcal{M}_k of marked elements $\tau \in \mathcal{T}_k$. Finally, the procedure ‘‘Refine’’ produces a new partition \mathcal{T}_{k+1} by refining all elements in \mathcal{M}_k at least once. Here we use a shape-regular bisection for the refinement. To keep the conformity, we usually partition a few more elements $\tau \in \mathcal{T}_k \setminus \mathcal{M}_k$.

Given a triangulation \mathcal{T}_h and the corresponding finite element solution (Λ_h, Φ_h) , we respectively define the element residual $\mathcal{R}_{\tau}(\Phi_h)$ and the jump $J_e(\Phi_h)$ by

$$\begin{aligned} \mathcal{R}_{\tau}(\Phi_h) &= \left(H_{\Phi_h} \phi_{i,h} - \sum_{j=1}^N \lambda_{ji,h} \phi_{j,h} \right)_{i=1}^N \quad \text{in } \tau \in \mathcal{T}_h, \\ J_e(\Phi_h) &= (j_e(\phi_{i,h}))_{i=1}^N, \quad j_e(\phi_{i,h}) = \kappa \nabla \phi_{i,h}|_{\tau_1} \cdot \vec{n}_1 + \kappa \nabla \phi_{i,h}|_{\tau_2} \cdot \vec{n}_2, \end{aligned}$$

where e is the common face of elements τ_1 and τ_2 with unit outward normals \vec{n}_1 and \vec{n}_2 . For $\tau \in \mathcal{T}_h$, we define the local error indicator $\eta_h(\Phi_h, \tau)$ as follows:

$$\eta_h^2(\Phi_h, \tau) = h_\tau^2 \|\mathcal{R}_\tau(\Phi_h)\|_{0,\tau}^2 + \sum_{e \in \mathcal{E}_h, e \subset \partial\tau} h_e \|J_e(\Phi_h)\|_{0,e}^2.$$

Depending on the a posteriori error indicators $\{\eta_k(\Phi_k, \tau)\}_{\tau \in \mathcal{T}_k}$, the procedure ‘‘Mark’’ gives a strategy to create a subset of elements \mathcal{M}_k of \mathcal{T}_k . Here, we consider ‘‘maximum strategy’’ which only requires that the set of marked elements \mathcal{M}_k contains at least one element of \mathcal{T}_k holding the largest value estimator. Namely, there exists at least one element $\tau_k^{\max} \in \mathcal{M}_k$ such that

$$\eta_k(\Phi_k, \tau_k^{\max}) = \max_{\tau \in \mathcal{T}_k} \eta_k(\Phi_k, \tau).$$

The adaptive finite element algorithm for solving (2.7) is stated as follows [7, 8, 10]:

Algorithm 1

1. Pick an initial mesh \mathcal{T}_0 and let $k = 0$.
 2. Solve (2.10) on \mathcal{T}_k to get the discrete ground state solution $(\lambda_{i,k}, \phi_{i,k})(i = 1, 2, \dots, N)$.
 3. Compute the local error indicators $\eta_k(\Phi_k, \tau)$ for all $\tau \in \mathcal{T}_k$.
 4. Construct $\mathcal{M}_k \subset \mathcal{T}_k$ by the maximum strategy.
 5. Refine \mathcal{T}_k to get a new conforming mesh \mathcal{T}_{k+1} .
 6. Let $k = k + 1$ and go to 2.
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We observe that there are a number of works on analyzing adaptive finite element methods in the literature. We refer to [4–6, 11, 15, 16] and references cited therein for linear eigenvalue problems and to [7, 8, 10] for nonlinear cases when the initial mesh is fine enough. We see that under the so-called Non-Degeneracy assumption¹, [14] proved the convergence of an adaptive finite element method starting from any initial mesh for some linear elliptic eigenvalue problems.

2.3. A polynomial theory

In our analysis, we need the following basic results, which are motivated by [36].

Lemma 2.1. *Let k be a prime number. Then there exist polynomials with respect to t_1, t_2, \dots, t_k*

$$\{p_j(t_1, t_2, \dots, t_k) : j = 2, \dots, k\}$$

with real coefficients satisfying

- (1) $p_j(t_1, t_2, \dots, t_k)$ is a polynomial of a degree not larger than $j - 1$ with respect to t_k and

$$p_j(\lambda t_1, \lambda t_2, \dots, \lambda t_{k-1}, t_k) = \lambda^j p_j(t_1, t_2, \dots, t_{k-1}, t_k) \quad \forall \lambda \in \mathbb{R};$$

- (2) if $\gamma, a_1, a_2, \dots, a_{k-1}, t \in \mathbb{R}$ satisfy $\gamma = a_1 t + a_2 t^2 + \dots + a_{k-1} t^{k-1}$, then

$$\gamma^k + \sum_{j=2}^k p_j(a_1, a_2, \dots, a_{k-1}, t^k) \gamma^{k-j} = 0.$$

¹No eigenfunction is equal to a polynomial of degree $\leq n$ on an open subset of Ω , where n denotes the polynomial degree of the finite element bases being used.

The proof of Lemma 2.1 is given in Appendix A.

Lemma 2.2. *Suppose k is a prime. Then for any positive integer n , there exist polynomials*

$$\{H_{n,j}(t_1, t_2, \dots, t_n) : j = 0, 1, 2, \dots, k^{n-1}\}$$

with real coefficients satisfying

(1) $H_{n,0}(t_1, t_2, \dots, t_n) = 1$, $H_{n,j}(t_1, t_2, \dots, t_n)$ ($j = 1, 2, \dots, k^{n-1}$) are homogeneous:

$$H_{n,j}(\lambda t_1, \lambda t_2, \dots, \lambda t_n) = \lambda^j H_{n,j}(t_1, t_2, \dots, t_n) \quad \forall \lambda \in \mathbb{R},$$

and $(-1)^{k^{n-1}} H_{n,k^{n-1}}(t_1, t_2, \dots, t_n)$ is a monic polynomial of a degree k^{n-1} with respect to each variable t_l ($l = 1, 2, \dots, n$);

(2) if $\gamma, t_1, t_2, \dots, t_n \in \mathbb{R}$ satisfy $\gamma = \sum_{j=1}^n t_j$, then

$$\sum_{j=0}^{k^{n-1}} H_{n,j}(t_1^k, t_2^k, \dots, t_n^k) \gamma^{k(k^{n-1}-j)} = 0.$$

Proof. We prove the conclusion by induction on n . First, for $n = 1$, $\gamma = t_1$ implies $\gamma^k - t_1^k = 0$, which shows that Lemma 2.2 is true when $n = 1$, namely, $H_{1,1}(t_1) = -t_1$. Assume that Lemma 2.2 is true for $n \geq 1$. We show that Lemma 2.2 is true for $n + 1$. Let

$$\sum_{j=1}^{n+1} t_j = \gamma.$$

It follows from the induction hypothesis and

$$\sum_{j=1}^n t_j = \gamma - t_{n+1}$$

that there exist polynomials

$$\{H_{n,j}(s_1, s_2, \dots, s_n) : j = 0, 1, 2, \dots, k^{n-1}\}$$

with real coefficients satisfying that $(-1)^{k^{n-1}} H_{n,k^{n-1}}(s_1, s_2, \dots, s_n)$ is a monic polynomial of a degree k^{n-1} with respect to each variable s_l ($l = 1, 2, \dots, n$), $H_{n,j}(s_1, s_2, \dots, s_n)$ ($j = 1, 2, \dots, k^{n-1}$) are homogeneous, and

$$\sum_{j=0}^{k^{n-1}} H_{n,j}(t_1^k, t_2^k, \dots, t_n^k) (\gamma - t_{n+1})^{k(k^{n-1}-j)} = 0.$$

We obtain from Newton binomial theory that

$$\sum_{i=1}^{k-1} a_i \gamma^k \left(-\frac{t_{n+1}}{\gamma} \right)^i = a, \quad (2.11)$$

where

$$\begin{aligned} a &= H_{n,k^{n-1}}(t_1^k, t_2^k, \dots, t_n^k) + (-t_{n+1})^{k^n} + \gamma^{k^n} + \sum_{\ell=1}^{k^{n-1}-1} \binom{k^n}{k\ell} \gamma^{k^n-k\ell} (-t_{n+1})^{k\ell} \\ &\quad + \sum_{j=1}^{k^{n-1}-1} H_{n,j}(t_1^k, t_2^k, \dots, t_n^k) \sum_{\ell=0}^{k^{n-1}-j} \binom{k^n-kj}{k\ell} \gamma^{k^n-kj-k\ell} (-t_{n+1})^{k\ell}, \\ a_i &= - \sum_{j=0}^{k^{n-1}-1} H_{n,j}(t_1^k, t_2^k, \dots, t_n^k) \sum_{\ell=1}^{k^{n-1}-j} \binom{k^n-kj}{k\ell-k+i} \gamma^{k^n-kj-k\ell} (-t_{n+1})^{k\ell-k}, \\ &\quad i = 1, 2, \dots, k-1. \end{aligned}$$

Let polynomials P and $P_i (i = 1, 2, \dots, k-1)$ be

$$\begin{aligned} P(s_1, s_2, \dots, s_{n+2}) &= H_{n, k^{n-1}}(s_1, s_2, \dots, s_n) + (-s_{n+1})^{k^{n-1}} + s_{n+2}^{k^{n-1}} + \sum_{\ell=1}^{k^{n-1}-1} \binom{k^n}{k\ell} s_{n+2}^{k^{n-1}-\ell} (-s_{n+1})^\ell \\ &\quad + \sum_{j=1}^{k^{n-1}-1} H_{n, j}(s_1, s_2, \dots, s_n) \sum_{\ell=0}^{k^{n-1}-j} \binom{k^n - kj}{k\ell} s_{n+2}^{k^{n-1}-j-\ell} (-s_{n+1})^\ell, \\ P_i(s_1, s_2, \dots, s_{n+2}) &= - \sum_{j=0}^{k^{n-1}-1} H_{n, j}(s_1, s_2, \dots, s_n) \sum_{\ell=1}^{k^{n-1}-j} \binom{k^n - kj}{k\ell - k + i} s_{n+2}^{k^{n-1}-j-\ell} (-s_{n+1})^{\ell-1}, \\ &\quad i = 1, 2, \dots, k-1. \end{aligned}$$

It is clear that P and $P_i (i = 1, 2, \dots, k-1)$ are homogeneous, $\deg P = k^{n-1}$, $\deg P_i = k^{n-1} - 1 (i = 1, 2, \dots, k-1)$, and

$$a = P(t_1^k, t_2^k, \dots, t_{n+1}^k, \gamma^k), \quad (2.12)$$

$$a_i = P_i(t_1^k, t_2^k, \dots, t_{n+1}^k, \gamma^k) \quad i = 1, 2, \dots, k-1. \quad (2.13)$$

Since k is a prime, we see from (2.11) that there exist $\{p_j(t_1, t_2, \dots, t_k) : j = 2, 3, \dots, k\}$ satisfying Lemma 2.1, namely,

$$0 = a^k + \sum_{j=2}^k p_j(a_1 \gamma^k, a_2 \gamma^k, \dots, a_{k-1} \gamma^k, (-t_{n+1})^k / \gamma^k) a^{k-j},$$

or

$$0 = a^k + \sum_{j=2}^k p_j(a_1, a_2, \dots, a_{k-1}, (-t_{n+1})^k / \gamma^k) \gamma^{kj} a^{k-j}. \quad (2.14)$$

We define $Q(s_1, s_2, \dots, s_{n+2})$ by

$$Q = P^k + \sum_{j=2}^k p_j(P_1, P_2, \dots, P_{k-1}, (-1)^k s_{n+1} / s_{n+2}) s_{n+2}^j P^{k-j}.$$

Thus it follows from (1) in Lemma 2.1 and (2.12), (2.13) that Q is a homogeneous polynomial of a degree k^n and

$$a^k + \sum_{j=2}^k p_j(a_1, a_2, \dots, a_{k-1}, (-t_{n+1})^k / \gamma^k) \gamma^{kj} a^{k-j} = Q(t_1^k, t_2^k, \dots, t_{n+1}^k, \gamma^k). \quad (2.15)$$

We see that Q can be expressed as

$$Q(s_1, s_2, \dots, s_{n+2}) = \sum_{j=0}^{k^n} H_{n+1, j}(s_1, s_2, \dots, s_{n+1}) s_{n+2}^{k^n-j}, \quad (2.16)$$

where $H_{n+1, j} (j = 1, 2, \dots, k^n)$ are homogeneous:

$$H_{n+1, j}(\lambda s_1, \lambda s_2, \dots, \lambda s_{n+1}) = \lambda^j H_{n+1, j}(s_1, s_2, \dots, s_{n+1}) \quad \forall \lambda \in \mathbb{R}.$$

It is not difficult to see that $H_{n+1, 0}(s_1, s_2, \dots, s_n) = 1$. We obtain from the definitions of P, P_i and Q that

$$\begin{aligned} &H_{n+1, k^n}(s_1, s_2, \dots, s_{n+1}) \\ &= \left(H_{n, k^{n-1}}(s_1, s_2, \dots, s_n) + (-s_{n+1})^{k^{n-1}} + \sum_{j=1}^{k^{n-1}-1} H_{n, j}(s_1, s_2, \dots, s_n) (-s_{n+1})^{k^{n-1}-j} \right)^k. \end{aligned}$$

Since $(-1)^{k^{n-1}} H_{n,k^{n-1}}(s_1, s_2, \dots, s_n)$ is a monic polynomial of a degree k^{n-1} with respect to each variable $s_l (l = 1, 2, \dots, n)$, we have that $(-1)^{k^n} H_{n+1,k^n}(s_1, s_2, \dots, s_{n+1})$ is a monic polynomial of a degree k^n with respect to each variable $s_l (l = 1, 2, \dots, n + 1)$. It follows from (2.14) to (2.16) that $H_{n+1,j} (j = 0, 1, \dots, k^n)$ satisfy (2) in Lemma 2.2. This completes the proof. \square

Since every integer larger than 1 can be written as a product of one or more primes, we arrive at

Proposition 2.3. *Let k and n be two positive integers. Then there exists a homogeneous polynomial $P(t_1, t_2, \dots, t_{n+1})$ with real coefficients satisfying*

- (1) *the degree of P with respect to each variable is the same;*
- (2) *P is a monic polynomial with respect to t_{n+1} ;*
- (3) *if $\gamma, t_1, t_2, \dots, t_n \in \mathbb{R}$ satisfy $\gamma = \sum_{j=1}^n t_j$, then*

$$P(t_1^k, t_2^k, \dots, t_n^k, \gamma^k) = 0.$$

Remark 2.4. Proposition 2.3 shows that there exists a real homogeneous polynomial P such that any zero of

$$p(t_1, t_2, \dots, t_n, \gamma) \equiv \sum_{i=1}^n \sqrt[k]{t_i} - \gamma$$

is a zero of

$$P(t_1, t_2, \dots, t_n, \gamma^k).$$

Proposition 2.5. *Let G be a nonempty open set of \mathbb{R}^3 . If $p \in \mathcal{P}_{\mathbb{Q}_+}(G)$ and $\deg p > 0$, then for any nonempty open set $G_0 \subset G$, there exists $x_0 \in G_0$ such that $p(x_0) \neq 0$.*

Proof. We see from the definition of $\mathcal{P}_{\mathbb{Q}_+}(G)$ that

$$p = \sum_{i=1}^n a_{\alpha^{(i)}} x^{\alpha^{(i)}},$$

where $\alpha^{(i)} \in \mathbb{Q}_+^3, 0 \neq a_{\alpha^{(i)}} \in \mathbb{R}$, and $\alpha^{(n)}$ is the max index. Hence we can choose a positive integer k such that all components of $k\alpha^{(i)} (i = 1, 2, \dots, n)$ are integers.

Assume that $p = 0$ in G_0 . Then there exists a real homogeneous polynomial $P(t_1, t_2, \dots, t_n)$ satisfying (2) of Proposition 2.3 and

$$P(x^{k\alpha^{(1)}}, x^{k\alpha^{(2)}}, \dots, x^{k\alpha^{(n)}}) = 0, \quad \text{in } G_0.$$

Set $Q = P(x^{k\alpha^{(1)}}, x^{k\alpha^{(2)}}, \dots, x^{k\alpha^{(n)}})$. Then Q is a polynomial with a positive degree which is a contradiction to $Q = 0$. This completes the proof. \square

Lemma 2.6. *Let $n \geq 2$ be a positive integer, G and G_0 be nonempty open subsets of \mathbb{R}^3 with $G_0 \subset G$. Let $p_j \in \mathcal{P}_{\mathbb{Q}_+}^{1/k}(G)$ for some positive integer k and $q_j \in \mathcal{P}_{\mathbb{Q}_+}(G) (j = 1, 2, \dots, n)$. If $q_j > 0 (j = 1, 2, \dots, n)$ in G_0 with $q_{j_0} \neq 1$ in G_0 for some j_0 and*

$$\deg p_{j_0} > \deg p_j \quad \forall j \in \{1, 2, \dots, n\} \setminus \{j_0\},$$

then there exists $x_0 \in G_0$ such that

$$\sum_{j=1}^n p_j(x_0) \ln q_j(x_0) \neq 0.$$

The proof of Lemma 2.6 is provided in Appendix B.

3. BEHAVIOR OF EIGENFUNCTION

In this section, we investigate the non-polynomial behavior of eigenfunctions of (1.1), which will be applied to analyze the convergence of their adaptive finite element approximations. We see from [17, 34] that the eigenfunctions of (1.1) vary rapidly around nuclei, which indeed results in applying adaptive finite element computations.

We first recall the unique continuation property.

Definition 3.1. Equation (1.1) has a unique continuation property if every solution in $H_{\text{loc}}^2(\Omega)$ that vanishes on an open set of Ω vanishes identically.

To look into if (1.1) has a unique continuation property, we may apply the following conclusion, which can be found in [33].

Lemma 3.2. Assume that $u \in H_{\text{loc}}^2(\Omega)$ and $\mathcal{V} \in L_{\text{loc}}^{3/2}(\Omega)$ such that $|\Delta u| \leq \mathcal{V}|u|$ a.e.. If u vanishes on an open set of Ω , then u is identically zero on Ω .

Theorem 3.3. If $V \in L^2(\Omega)$ and $\mathcal{N}_1(t) \in \mathcal{P}(s, (c_1, c_2))$ with $s \in [0, 3/2]$, then (1.1) has a unique continuation property.

Proof. It follows from a standard elliptic regularity argument that $\phi_i \in H^2(\Omega)$ (see, e.g., [17, 34] and Sect. 4.3.1 of [23]), which together with Sobolev imbedding theorem leads to $\phi_i \in C(\bar{\Omega})$ ($i = 1, 2, \dots, N$).

Note that Young's inequality and Sobolev imbedding theorem imply

$$\|\mathcal{N}_2(\rho)\|_{0,\infty,\Omega} \leq C\|\rho\|_{0,\Omega} \leq C \sum_{i=1}^N \|\phi_i\|_{0,4,\Omega}^2 \leq C\|\Phi\|_{1,\Omega}^2 < \infty.$$

We have that $|\Delta \phi_i| = \mathcal{V}_i |\phi_i|$ and $\mathcal{V}_i \in L_{\text{loc}}^{3/2}(\Omega)$, where $\mathcal{V}_i = |V + \mathcal{N}(\rho) - \lambda_i|/\kappa$ ($i = 1, 2, \dots, N$). Thus we arrive at the conclusion from Lemma 3.2. \square

Remark 3.4. We may see from the proof of Theorem 3.3 that if $V \in L^2(\Omega)$ is replaced by $V \in L_{\text{loc}}^{3/2}(\Omega)$ and any solution of (1.1) is in $H^2(\Omega)$, then (1.1) has a unique continuation property.

Theorem 3.5. Let $\Phi = (\phi_1, \phi_2, \dots, \phi_N)$ be a solution of (1.1). Assume that V and \mathcal{N} are defined by (2.1) and (2.2)–(2.4) with $\alpha = 0$, respectively. If V is a non-constant function and

$$\deg p_1 - \deg h_1 > \max \left\{ 0, \max_{1 \leq j \leq M} (\deg f_j - \deg g_j)/2, \max_{2 \leq i \leq K} (\deg p_i - \deg h_i) \right\}, \quad (3.1)$$

then for any nonempty open set $G \subset \Omega$, there exists an eigenfunction ϕ_j ($j \in \{1, 2, \dots, N\}$) being not a non-zero polynomial on G . If in addition, $V \in L^2(\Omega)$ and $\mathcal{N}_1(t) \in \mathcal{P}(s, (c_1, c_2))$ with $s \in [0, 3/2]$, then for any nonempty open set $G \subset \Omega$, there exists an eigenfunction ϕ_j ($j \in \{1, 2, \dots, N\}$) being not a polynomial on G .

Proof. Assume that all eigenfunctions $\{\phi_1, \phi_2, \dots, \phi_N\}$ are polynomials on the nonempty open set G : $\phi_j \in \mathcal{P}_\ell(G)$ ($j = 1, 2, \dots, N$) for some positive integer ℓ . Without loss of generality, let $\deg \phi_1 \geq \max_{2 \leq j \leq N} \deg \phi_j$. We have $\deg \rho = 2 \deg \phi_1$ and see from (1.1) that

$$-\kappa \Delta \phi_1 - \sum_{j=1}^M \frac{f_j}{g_j} \phi_1 + \sum_{i=1}^K \frac{p_i(\rho)}{h_i(\rho)} \phi_1 \ln q_i(\rho) = \lambda_1 \phi_1, \quad \text{in } G. \quad (3.2)$$

If $\deg \phi_1 > 0$, then we see from (3.1) that

$$\begin{aligned} (\deg p_1 - \deg h_1) \deg \rho + \deg \phi_1 &> \deg \Delta \phi_1, \\ (\deg p_1 - \deg h_1) \deg \rho + \deg \phi_1 &> \deg \left(\frac{f_j}{g_j} \phi_1 \right), & j = 1, 2, \dots, N, \\ (\deg p_1 - \deg h_1) \deg \rho + \deg \phi_1 &> (\deg p_i - \deg h_i) \deg \rho + \deg \phi_1, & i = 2, 3, \dots, K, \\ (\deg p_1 - \deg h_1) \deg \rho + \deg \phi_1 &> \deg \phi_1. \end{aligned}$$

Since q_i are polynomials implying $q_i(\rho) \in \mathcal{P}_{\mathbb{Q}_+}(\Omega) (i = 1, 2, \dots, K)$, we obtain from Lemma 2.6 that

$$-\kappa \Delta \phi_1(x_0) - \sum_{j=1}^M \frac{f_j(x_0)}{g_j(x_0)} \phi_1(x_0) + \sum_{i=1}^K \frac{p_i(\rho)(x_0)}{h_i(\rho)(x_0)} \phi_1(x_0) \ln q_i(\rho)(x_0) \neq \lambda_1 \phi_1(x_0)$$

for some $x_0 \in G$, which is a contradiction to (3.2). Thus we arrive at that $\deg \phi_1 = 0$ on G . Since $\deg \phi_1 \geq \max_{2 \leq j \leq N} \deg \phi_j$, we have that $\phi_j = c_j (j = 1, 2, \dots, N)$ are constants on G . If $c_j \neq 0$ for all $j \in \{1, 2, \dots, N\}$, then

$$\sum_{j=1}^M \frac{f_j}{g_j} = \sum_{i=1}^K \frac{p_i(\rho)}{h_i(\rho)} \ln q_i(\rho) - \lambda_1, \quad \text{in } G,$$

with the constant $\rho = \sum_{j=1}^N c_j^2$, which is impossible. Hence $c_j = 0$ for some $j \in \{1, 2, \dots, N\}$.

If in addition, $V \in L^2(\Omega)$ and $\mathcal{N}_1(t) \in \mathcal{P}(s, (c_1, c_2))$ with $s \in [0, 3/2]$, then Theorem 3.3 implies that $\phi_j = 0$ in Ω for some $j \in \{1, 2, \dots, N\}$, which is a contradiction to $\int_{\Omega} \phi_j^2 = 1$. This completes the proof. \square

Remark 3.6. We see from the above conclusion that the eigenfunction cannot be a polynomial on any open set when $N = 1$.

Remark 3.7. Note that Theorem 3.5 may be also true even if

$$\deg p_1 - \deg h_1 = \max_{1 \leq j \leq M} (\deg f_j - \deg g_j) / 2.$$

For instance, no eigenfunction $\phi \in H^2(\Omega)$ of GPE [2, 35]

$$\left(-\frac{1}{2} \Delta + V + \beta |\phi|^2 \right) \phi = \lambda \phi$$

with a harmonic trap potential

$$V(x) = \gamma_1 \xi_1^2 + \gamma_2 \xi_2^2 + \gamma_3 \xi_3^2, \quad \gamma_1, \gamma_2, \gamma_3 > 0$$

can be a polynomial on any open set $G \subset \Omega$, where $x = (\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3$.

Theorem 3.8. Let $\Phi = (\phi_1, \phi_2, \dots, \phi_N)$ be a solution of (1.1). Assume that V and \mathcal{N} are defined by (2.1) and (2.2)–(2.4) with $\alpha \neq 0$, respectively, and $\alpha \Delta V$ is not a positive constant function. If either of the following conditions holds:

(1)

$$\max_{1 \leq i \leq K} (\deg p_i - \deg h_i) \leq 1 \quad \text{and} \quad \max_{1 \leq j \leq M} (\deg f_j - \deg g_j) < 4,$$

(2) $\deg q_1 = 0$ and

$$\deg p_1 - \deg h_1 > \max \left\{ 2, \max_{1 \leq j \leq M} (\deg f_j - \deg g_j) / 2, \max_{2 \leq i \leq K} (\deg p_i - \deg h_i) \right\}, \quad (3.3)$$

then for any nonempty open set $G \subset \Omega$, there exists an eigenfunction $\phi_j (j \in \{1, 2, \dots, N\})$ being not a non-zero polynomial on G . If in addition, $V \in L^2(\Omega)$ and $\mathcal{N}_1(t) \in \mathcal{P}(s, (c_1, c_2))$ with $s \in [0, 3/2]$, then for any nonempty open set $G \subset \Omega$, there exists an eigenfunction $\phi_j (j \in \{1, 2, \dots, N\})$ being not a polynomial on G .

Proof. Assume that all eigenfunctions $\{\phi_1, \phi_2, \dots, \phi_N\}$ are polynomials on nonempty open set G : $\phi_j \in \mathcal{P}_\ell(G) (j = 1, 2, \dots, N)$ for some positive integer ℓ . Without loss of generality, let $\deg \phi_1 \geq \max_{2 \leq j \leq N} \deg \phi_j$. Obviously, $\deg \rho = 2 \deg \phi_1$.

If $\phi_1(x) \neq 0$ for any $x \in G$ and $\deg \phi_1 > 0$, then we obtain from (1.1) that

$$-\kappa \frac{\Delta \phi_1}{\phi_1} - \sum_{j=1}^M \frac{f_j}{g_j} + \alpha \int_{\Omega} \frac{\rho(y)}{|\cdot - y|} dy + \sum_{i=1}^K \frac{p_i(\rho)}{h_i(\rho)} \ln q_i(\rho) = \lambda_1, \quad \text{in } G.$$

Applying the Laplace operator to both sides yields

$$-\kappa p_{\phi_1} - \sum_{j=1}^M f_{j,g} - 4\alpha\pi\rho + \sum_{i=1}^K p_{i,h,\rho} \ln q_i(\rho) + \sum_{i=1}^K p_{i,h,q,\rho} = 0, \quad \text{in } G, \tag{3.4}$$

where

$$\begin{aligned} p_{\phi_1} &= \Delta \left(\frac{\Delta \phi_1}{\phi_1} \right), \\ f_{j,g} &= \Delta \left(\frac{f_j}{g_j} \right), \quad j = 1, \dots, M, \\ p_{i,h,\rho} &= \Delta \left(\frac{p_i(\rho)}{h_i(\rho)} \right), \quad i = 1, \dots, K, \\ p_{i,h,q,\rho} &= 2 \frac{\nabla(p_i(\rho)/h_i(\rho)) \cdot \nabla q_i(\rho)}{q_i(\rho)} + \frac{p_i(\rho)(q_i(\rho)\Delta q_i(\rho) - |\nabla q_i(\rho)|^2)}{h_i(\rho)q_i^2(\rho)}, \quad i = 1, \dots, K. \end{aligned}$$

If $\max_{1 \leq i \leq K} (\deg p_i - \deg h_i) \leq 1$ and $\max_{1 \leq j \leq M} (\deg f_j - \deg g_j) < 4$, then only $4\alpha\pi\rho$ has the max degree.

If $\deg q_1 = 0$ and (3.3) holds, then $p_{1,h,q,\rho} = 0$. Thus only one term, which is one term of $p_{1,h,\rho}$, has the max degree.

Therefore, we get a contradiction to (3.4) from Lemma 2.6. Consequently, $\deg \phi_1 \geq \max_{2 \leq j \leq N} \deg \phi_j$ leads to that $\phi_j = c_j (j = 1, 2, \dots, N)$ are constants in G .

If $c_j \neq 0$ for all $j \in \{1, 2, \dots, N\}$, we then derive from (3.4) that

$$\Delta V = 4\alpha\pi \sum_{i=1}^N c_i^2 \quad \forall x \in G,$$

which is impossible. Hence $c_j = 0$ for some $j \in \{1, 2, \dots, N\}$.

If in addition, $V \in L^2(\Omega)$ and $\mathcal{N}_1(t) \in \mathcal{P}(s, (c_1, c_2))$ with $s \in [0, 3/2]$, then we complete the proof by using Theorem 3.3. □

We may apply Theorem 3.5 or Theorem 3.8 to the typical mathematical models in quantum physics to see the eigenfunction behavior. The following are some examples.

Example 3.9. No eigenfunction of the Schrödinger–Newton equation [18]

$$\left(-\Delta - \int_{\Omega} \frac{|u(y)|^2}{|\cdot - y|} dy \right) u = \lambda u, \quad \text{in } \mathbb{R}^3$$

can be a polynomial on any open set of \mathbb{R}^3 .

Example 3.10. No eigenfunction of the Thomas–Fermi–Dirac–von Weizsäcker equation [7, 21]

$$\left(-\kappa\Delta - \sum_{j=1}^M \frac{Z_j}{|\cdot - r_j|} + \int_{\Omega} \frac{|u(y)|^2}{|\cdot - y|} dy + \beta_1 u^{2\nu-2} - \beta_2 u^{2/3} \right) u = \lambda u$$

can be a polynomial locally for a rational number ν in $[1, 2]$, where β_1 and β_2 are constants.

Example 3.11. The Kohn–Sham equation of a system consisting of M nuclei of charges $\{Z_1, Z_2, \dots, Z_M\}$ located at the positions $\{r_1, r_2, \dots, r_M\}$ and N electrons is as follows:

$$\begin{cases} \left(-\frac{1}{2}\Delta + V_{\text{ext}} + \int_{\Omega} \frac{\rho(y)}{|\cdot - y|} dy + V_{\text{xc}}(\rho) \right) \phi_i = \lambda_i \phi_i, & \text{in } \Omega, \quad i = 1, 2, \dots, N, \\ \int_{\Omega} \phi_i \phi_j = \delta_{ij}, \end{cases} \quad (3.5)$$

where $V_{\text{ext}} = -\sum_{k=1}^M \frac{Z_k}{|\cdot - r_k|}$ is the associated external potential, $\rho = \sum_{i=1}^N |\phi_i|^2$ is the electronic density, and $V_{\text{xc}}(\rho)$ is the exchange-correlation potential such as the X_{α} exchange-correction potential [30]

$$V_{\text{xc}}(\rho) = \frac{3}{2}\alpha \left(\frac{3}{\pi\rho} \right)^{1/3} \quad (3.6)$$

with $\alpha \in [2/3, 1]$ or the Perdew–Zunger type local-density approximations (LDA) potential [26]:

$$V_{\text{xc}}^{\text{LDA}}(\rho) = \begin{cases} -\frac{0.1423 + 0.0633r_s + 0.1748\sqrt{r_s}}{(1 + 1.0529\sqrt{r_s} + 0.3334r_s)^2} - \left(\frac{9}{4\pi^2} \right)^{\frac{1}{3}} \frac{1}{r_s}, & \text{if } r_s \geq 1, \\ 0.0311 \ln r_s - 0.0584 + 0.0013r_s \ln r_s - 0.0084r_s - \left(\frac{9}{4\pi^2} \right)^{\frac{1}{3}} \frac{1}{r_s}, & \text{if } r_s < 1 \end{cases} \quad (3.7)$$

with $r_s = \left(\frac{3}{4\pi\rho} \right)^{1/3}$. It is clear that V_{ext} can be rewritten as the form (2.1). And (3.6) and (3.7) can be rewritten as the form (2.3).

We see that if the exchange-correction potential is chosen as either (3.6) or (3.7), then for any nonempty open set $G \subset \Omega$, there exists an eigenfunction ϕ_j ($j \in \{1, 2, \dots, N\}$) being not a polynomial on G .

In fact, the same conclusion is true for the Vosko–Wilk–Nusair type LDA potential [32]

$$V_{\text{xc}}(\rho) = \frac{A}{2} \left\{ \ln \frac{t^2}{X(t)} + \frac{2b}{Q} \tan^{-1} \frac{Q}{2t+b} - \frac{bt_0}{X(t_0)} \left(\ln \frac{(t-t_0)^2}{X(t)} + \frac{2(b+2t_0)}{Q} \tan^{-1} \frac{Q}{2t+b} \right) \right\},$$

where $r_s = \left(\frac{3}{4\pi\rho} \right)^{1/3}$, $t = r_s^{1/2}$, $X(t) = t^2 + bt + c$, $Q = (4c - b^2)^{1/2}$, $A = 0.0621814$, $t_0 = -0.409286$, $b = 13.0720$, and $c = 42.7198$.

Indeed, we conjecture that no eigenfunction of (1.1) can be a polynomial on any open set in \mathbb{R}^3 when $N > 1$. Unfortunately, it is still open whether it is true or not.

4. ADAPTIVE APPROXIMATIONS

In this section, we apply the behavior of the eigenfunctions to investigate the convergence of adaptive finite element approximations of (1.1). We assume that

- (i) $V \in L^2(\Omega)$;
- (ii) $\mathcal{E} \in \mathcal{P}(3, (c_1, c_2))$ with $c_1 \geq 0$ or $\mathcal{P}(4/3, (c_1, c_2))$;
- (iii) $\mathcal{N}_1 \in \mathcal{P}(s_1, (c_1, c_2))$ for some $s_1 \in [0, 2)$ and $t\mathcal{N}'(t) \in \mathcal{P}(s_2, (\tilde{c}_1, \tilde{c}_2))$ for some $s_2 \in [0, 2)$.

Let

$$\Omega^+ = \bigcup_{T \in \mathcal{T}^+} T,$$

where

$$\mathcal{T}^+ = \bigcup_{k \geq 0} \bigcap_{m \geq k} \mathcal{T}_m.$$

In our analysis, we need Lemma 4.3 in [14], which is stated as follows:

Lemma 4.1. *The set Ω^+ is empty if and only if $\lim_{k \rightarrow \infty} \|h_k\|_{0, \infty, \Omega} = 0$.*

Under the assumptions (i)–(iii), we observe from Theorem 3.5 in [10] and Theorem 4.2 in [7] that approximations Θ_k produced by Algorithm 1 converge to a solution of (1.1) for any initial mesh and the solution becomes a ground state if the initial mesh size is sufficiently small so that Θ_0 is sufficiently near to Θ . Indeed, based on the eigenfunction behavior, we are able to prove that Θ_k produced by Algorithm 1 converge to a ground state of (1.1) starting from any initial mesh under some assumptions.

Using the similar argument to the proof of Lemma 6.2 in [14], we have

Lemma 4.2. *Let mesh size functions $\{h_k\}_{k \in \mathbb{N}}$ and ground state solutions $\{\Theta_k = (\Lambda_k, \Phi_k)\}_{k \in \mathbb{N}}$ be produced by Algorithm 1. If for any nonempty open set $G \subset \Omega$, there exists an eigenfunction of (1.1) being not a polynomial on G , then $\|h_k\|_{0, \infty, \Omega} \rightarrow 0$ as $k \rightarrow \infty$.*

Proof. If $\|h_k\|_{0, \infty, \Omega}$ does not tend to zero, then we derive from Lemma 4.1 that Ω^+ is not empty. Thus there exists $T \in \mathcal{T}^+$ and $k_0 \in \mathbb{N}$ such that $T \in \mathcal{T}_k$ for all $k \geq k_0$.

Without loss of generality, we assume that ϕ_1 is not a polynomial on the nonempty open set T . We obtain from the proof of Theorem 3.5 in [10] that there exists a subsequence Φ_{k_m} and some solution Φ of (1.1) such that $\Phi_{k_m} \rightarrow \Phi$ in \mathcal{H} . Thus we have that $\phi_{1, k_m} \rightarrow \phi_1$ in $H_0^1(\Omega)$ as $m \rightarrow \infty$, which derives

$$\lim_{m \rightarrow \infty} \|\phi_{1, k_m} - \phi_1\|_{0, T} = 0. \quad (4.1)$$

Combining (4.1), $\phi_{1, k}|_T \in \mathcal{P}_n(T)$ for some integer n , and that $\mathcal{P}_n(T)$ is a finite dimensional space, we obtain that $\phi_1 \in \mathcal{P}_n(T)$, which contradicts to that ϕ_1 is not a polynomial on T . This completes the proof. \square

Let the distance between sets $X, Y \subset \mathbb{R}^{N \times N} \times \mathcal{H}$ be defined by

$$d_{\mathcal{H}}(X, Y) = \sup_{(\Lambda, \Phi) \in X} \inf_{(\Sigma, \Psi) \in Y} (|\Lambda - \Sigma| + \|\Phi - \Psi\|_{1, \Omega}),$$

where $|\cdot|$ is the Frobenius norm in $\mathbb{R}^{N \times N}$.

To carry out the convergence analysis, the gap-condition

$$\min_{\Psi \in \mathcal{Q}} E(\Psi) < \inf_{(M, \Psi) \in \mathcal{W} \setminus \Theta} E(\Psi) \quad (4.2)$$

is assumed in [7, 10]. Consequently, we have

$$\min_{\Psi_h \in V_h \cap \mathcal{Q}} E(\Psi_h) < \inf_{(M, \Psi) \in \mathcal{W} \setminus \Theta} E(\Psi) \quad (4.3)$$

when h is small enough. In order to ensure (4.3), we observe that the initial mesh size h is assumed to be sufficiently small in [7, 10] (see [10], Thm. 3.5 and [7], Thm. 4.2). On the one hand, combining Theorems 3.5, 3.8, and Lemma 4.2, we indeed have that the mesh size h_k tends to zero under the assumption in Theorem 3.5 or that in Theorem 3.8, which shows that the mesh size h_k will be sufficiently small after finite iteration steps and hence (4.3) holds provided $k \gg 1$. Namely, we have

$$E(\Phi_k) < \inf_{(M, \Psi) \in \mathcal{W} \setminus \Theta} E(\Psi)$$

provided $k \gg 1$. On the other hand, we see that for any subsequence $\{(\Lambda_{k_m}, \Phi_{k_m})\}_{m \in \mathbb{N}}$, there exists a convergent subsequence $\{(\Lambda_{k_{m_j}}, \Phi_{k_{m_j}})\}_{j \in \mathbb{N}}$ and $(\Lambda_\infty, \Phi_\infty) \in \mathcal{W}$ such that $(\Lambda_{k_{m_j}}, \Phi_{k_{m_j}}) \rightarrow (\Lambda_\infty, \Phi_\infty)$ (see the proofs of Thm. 3.5 in [10] and Thm. 4.2 in [7] for more details). Hence we have $(\Lambda_\infty, \Phi_\infty) \in \Theta$ and arrive at

Theorem 4.3. *Let $\{\Theta_k\}_{k \in \mathbb{N}}$ be the sequence generated by Algorithm 1. If the gap-condition (4.2) and the assumption in Theorem 3.5 or that in Theorem 3.8 are satisfied, then*

$$\begin{aligned} \lim_{k \rightarrow \infty} E_k &= \min_{\Psi \in \Theta} E(\Psi), \\ \lim_{k \rightarrow \infty} d_{\mathcal{H}}(\Theta_k, \Theta) &= 0, \end{aligned}$$

where $E_k = E(\Phi)$ $((\Lambda, \Phi) \in \Theta_k)$.

Remark 4.4. We mention that we do not require the assumption in Theorem 4.3 that the ground state solution and the discrete ground state solution correspond to the lowest N eigenpairs of (2.7) and (2.10), respectively. In practice, however, Θ and Θ_h are assumed to be the lowest N eigenpairs of (2.7) and (2.10), respectively [22].

As a result, we see from [8, 10] that the adaptive finite element method has the asymptotic linear convergence rate and the asymptotic optimal complexity from any initial mesh. More precisely, the adaptive finite element method has the linear convergence rate and the optimal complexity after finite iteration steps.

5. CONCLUDING REMARKS

In this paper, we have investigated a class of nonlinear eigenvalue problems modeling quantum physics. We have first proved that for any open set G , there exists an eigenfunction that cannot be a polynomial on G , which may be reviewed as a refinement of the standard unique continuation property. Then applying the non-polynomial behavior of eigenfunctions, we have shown that adaptive finite element approximations converge to some ground state even if the initial mesh is not fine.

We mention that the same conclusion can be expected for any dimensions larger than 3. For instance, our arguments can be applied to the following linear eigenvalue problem:

$$-\nabla \cdot (\mathcal{A} \nabla u) + \mathcal{V}u = \lambda \mathcal{B}u, \quad \text{in } \Omega, \tag{5.1}$$

where $\Omega \subset \mathbb{R}^d$ for some positive integer $d \geq 3$ and \mathcal{A} is a symmetric-matrix-valued function and is uniformly positive definite. We see that (5.1) includes the electronic Schrödinger equation

$$\left(-\sum_{i=1}^N \frac{\hbar^2}{2m_e} \nabla_{x_i}^2 - \sum_{i=1}^N \sum_{j=1}^M \frac{Z_j e^2}{|x_i - r_j|} + \frac{1}{2} \sum_{i,j=1, i \neq j}^N \frac{e^2}{|x_i - x_j|} \right) \phi = E\phi, \quad \text{in } \mathbb{R}^{3N}, \tag{5.2}$$

where \hbar is the Planck's constant divided by 2π , m_e is the mass of the electron, $\{x_i : i = 1, \dots, N\}$ are variables that describe the electron positions, and e is the electronic charge, ϕ is the wavefunction, N is the number of electrons, M is the number of atoms, Z_j is the atomic number of the j -th atom, and r_j is the position of the j -th atom.

For convenience, we introduce the following assumptions:

- I Entries of \mathcal{A} are continuous and piecewise functions in $\mathcal{P}_{\mathbb{Q}_+}(\Omega)$.
- II \mathcal{B} is a piecewise function in $\mathcal{P}_{\mathbb{Q}_+}(\Omega)$.
- III $\mathcal{V} = -\sum_{j=1}^M \frac{f_j}{g_j}$, where f_j, g_j ($j = 1, 2, \dots, M$) are piecewise functions in $\mathcal{P}_{\mathbb{Q}_+}^\mu(\Omega)$ for some $\mu \in \mathbb{Q}_+$.
- IV \mathcal{V} cannot be equal to $\lambda\mathcal{B}$ for any $\lambda \in \mathbb{R}$ in any open subset of Ω .

If Assumptions I–IV hold true and that the entries of $\mathcal{A}|_G, \mathcal{B}|_G$ belong to $\mathcal{P}_{\mathbb{Q}_+}(G)$ and $f_j|_G, g_j|_G \in \mathcal{P}_{\mathbb{Q}_+}^\mu(G)$ for all $j \in \{1, 2, \dots, M\}$ imply that only one among $\deg \mathcal{A}|_G - 2, \deg \mathcal{B}|_G, \deg f_1|_G - \deg g_1|_G, \dots, \deg f_M|_G - \deg g_M|_G$ equals to

$$\max \{ \deg \mathcal{A}|_G - 2, \deg f_1|_G - \deg g_1|_G, \dots, \deg f_M|_G - \deg g_M|_G, \deg \mathcal{B}|_G \}$$

when $G \subset \Omega$ is an open subset, then no eigenfunction of (5.1) can be a non-zero polynomial on G . If in addition, (5.1) has a unique continuation property (see, *e.g.*, [29, 33]), then any H_{loc}^2 -eigenfunction of (5.1) cannot be a polynomial on any open subset of Ω . Since (5.2) satisfies Assumptions I–IV, in particular, we obtain the more sophisticate conclusion than that in the existing literature (see, *e.g.*, [28]).

Note that the so-called Non-Degeneracy Assumption of a linear case of

$$-\nabla \cdot (\mathcal{A}\nabla u) = \lambda\mathcal{B}u \tag{5.3}$$

has been introduced in [14], which is a special case of (5.1) when $\mathcal{V} = 0$, the entries of \mathcal{A} are continuous and piecewise linear, and \mathcal{B} is piecewise constant, with which together the convergence of an adaptive finite element method from any initial mesh for (5.3) is then derived.

APPENDIX A.

In this appendix, we provide a proof of Lemma 2.1, whose idea is inspired by Appendixes A and B of [27].

Proof. Let $\gamma = a_1t + a_2t^2 + \dots + a_{k-1}t^{k-1}$ with $\gamma, a_1, a_2, \dots, a_{k-1}, t \in \mathbb{R}$. For convenience, we may view γ as a polynomial $\gamma(t)$ with respect to t . Let $z \neq 1$ be a k th root of 1. We have

$$\sum_{j=0}^{k-1} z^j = 0 \tag{A.1}$$

and

$$\{z^{mj} : j = 1, 2, \dots, k-1\} = \{z^j : j = 1, 2, \dots, k-1\} \tag{A.2}$$

for any positive integer m that is not divisible by k . Let

$$P_t(y) = \prod_{m=0}^{k-1} (y - \gamma(z^m t)), \quad y \in \mathbb{R}, \tag{A.3}$$

we obtain that $P_t(\gamma) = 0$ since $z^0 = 1$. We claim that $P_t(\gamma) = 0$ yields the conclusion.

Indeed, it follows from (A.3) that $P_t(y)$ can be rewritten as

$$P_t(y) = y^k + \sum_{j=1}^k q_j(a_1, a_2, \dots, a_{k-1}, t)y^{k-j}, \tag{A.4}$$

where

$$q_j(t_1, t_2, \dots, t_k) = \sum_{\ell=j}^{j(k-1)} f_{j,\ell}(t_1, t_2, \dots, t_{k-1})t_k^\ell \tag{A.5}$$

for all $t_1, t_2, \dots, t_k \in \mathbb{R}$ and $f_{j,\ell}$ is either a zero polynomial or a homogeneous polynomial of a degree j for any $\ell = j, j+1, \dots, j(k-1)$. We see from (A.3) that $\bar{P}_t(y) = P_t(y)$. Thus q_j ($j = 1, 2, \dots, k$) are real polynomials. We obtain from (A.3) to (A.5) that

$$\begin{aligned} P_t(y) &= \frac{1}{k} \sum_{m=0}^{k-1} P_{z^m t}(y) = y^k + \sum_{j=1}^k \left(\frac{1}{k} \sum_{m=0}^{k-1} q_j(a_1, a_2, \dots, a_{k-1}, z^m t) \right) y^{k-j} \\ &= y^k + \sum_{j=1}^k \left(\frac{1}{k} \sum_{\ell=j}^{j(k-1)} f_{j,\ell}(a_1, a_2, \dots, a_{k-1}) t^\ell \sum_{m=0}^{k-1} z^{\ell m} \right) y^{k-j}, \end{aligned}$$

which together with (A.1) and (A.2) leads to

$$P_t(y) = y^k + \sum_{j=2}^k \left(\sum_{m=1}^{j-1} f_{j,mk}(a_1, a_2, \dots, a_{k-1}) t_k^m \right) y^{k-j}. \quad (\text{A.6})$$

Comparing (A.4) with (A.6), we arrive at

$$\begin{aligned} q_1(t_1, t_2, \dots, t_k) &= 0, \\ q_j(t_1, t_2, \dots, t_k) &= \sum_{m=1}^{j-1} f_{j,mk}(t_1, t_2, \dots, t_{k-1}) t_k^m, \quad j = 2, \dots, k \end{aligned} \quad (\text{A.7})$$

for all $t_1, t_2, \dots, t_k \in \mathbb{R}$. Let

$$p_j(t_1, t_2, \dots, t_k) = \sum_{m=1}^{j-1} f_{j,mk}(t_1, t_2, \dots, t_{k-1}) t_k^m, \quad j = 2, \dots, k,$$

then we have

$$q_j(t_1, t_2, \dots, t_k) = p_j(t_1, t_2, \dots, t_{k-1}, t_k^k), \quad j = 2, 3, \dots, k. \quad (\text{A.8})$$

Thus we complete the proof by using $P_t(\gamma) = 0$, (A.7), (A.8), and that $f_{j,\ell}$ is either a zero polynomial or homogeneous of a degree j for any ℓ . \square

APPENDIX B.

In this appendix, we provide a proof of Lemma 2.6.

Proof. Without loss of generality, we divide n into two parts: $n = n_1 + n_2$, such that $\deg q_j = 0$ for $j \in \{1, \dots, n_1\}$ and $\deg q_j > 0$ for $j \in \{n_1 + 1, \dots, n_1 + n_2\}$.

We prove the conclusion by induction on n_2 .

(1) For $n_2 = 0$, we prove the conclusion by contradiction again. Assume that

$$\sum_{j=1}^{n_1} p_j \ln q_j = 0, \quad \text{in } G_0,$$

where $\ln q_j$ are constants and $\ln q_{j_0}(x) \neq 0$ for any $x \in G_0$.

For convenience, we assume $j_0 = 1$. Let $P(t_1, t_2, \dots, t_{n_1})$ be a real homogeneous polynomial satisfying (2) of Proposition 2.3 and

$$P(p_2^k, \dots, p_{n_1}^k, p_1^k) = 0, \quad \text{in } G_0.$$

Set $Q = P(p_2^k, \dots, p_n^k, p_1^k)$. We get from $p_j \in \mathcal{P}_{\mathbb{Q}_+}^{1/k} (j = 1, 2, \dots, n_1)$ that $Q \in \mathcal{P}_{\mathbb{Q}_+}$. Note that P is a homogeneous polynomial and monic in t_{n_1} , we obtain from the definition of Q and $\deg p_1 > \max_{2 \leq j \leq n_1} \deg p_j$ that $\deg Q > 0$. Therefore Proposition 2.5 leads to a contradiction to $Q = 0$ in G_0 . Thus Lemma 2.6 is true for $n_2 = 0$.

(2) Assume that Lemma 2.6 is true for $n_2 \geq 0$. We show that Lemma 2.6 is true for $n_2 + 1$. Let $j_0 = 1$ or $j_0 = n_1 + 1$. It is obvious that the conclusion is true if $p_{n_1+1} = 0$ in G_0 . If $p_{n_1+1} \neq 0$ in G_0 , then we assume that

$$\sum_{j=1}^{n_1} p_j \ln q_j + \sum_{j=n_1+1}^{n_1+n_2+1} p_j \ln q_j = 0, \quad \text{in } G_0,$$

which leads to

$$\sum_{j=1}^{n_1} \frac{p_j}{p_{n_1+1}} \ln q_j + \ln q_{n_1+1} + \sum_{j=n_1+2}^{n_1+n_2+1} \frac{p_j}{p_{n_1+1}} \ln q_j = 0, \quad \text{in } \tilde{G} \tag{B.1}$$

for some nonempty open subset $\tilde{G} \subset G_0$, where $q_j (j = 1, \dots, n_1)$ are constants. Applying ∂_i to (B.1) ($i = 1, 2, 3$), we obtain

$$\sum_{j=1}^{n_1} \frac{\tilde{p}_{j,i}}{p_{n_1+1}^2} \ln q_j + \sum_{j=n_1+2}^{n_1+n_2+1} \frac{p_j \partial_i q_j}{p_{n_1+1} q_j} + \frac{\partial_i q_{n_1+1}}{q_{n_1+1}} + \sum_{j=n_1+2}^{n_1+n_2+1} \frac{\tilde{p}_{j,i}}{p_{n_1+1}^2} \ln q_j = 0, \quad \text{in } \tilde{G},$$

where $\tilde{p}_{j,i} = p_{n_1+1} \partial_i p_j - p_j \partial_i p_{n_1+1}$, $j = 1, \dots, n_1 + n_2 + 1$, $i = 1, 2, 3$. It is easy to see that $p_{n_1+1}^k p_j^k \xi_i \tilde{p}_{j,i} \in \mathcal{P}_{\mathbb{Q}_+}^{1/k}$.

If $j_0 = 1$, then there exists i such that $\deg \tilde{p}_{1,i} = \deg p_1 + \deg p_{n_1+1} - 1$. Thus we have

$$\begin{aligned} \deg \tilde{p}_{1,i} - \deg p_{n_1+1}^2 &> \deg \tilde{p}_{j,i} - \deg p_{n_1+1}^2, & j = 2, \dots, n_1 + n_2 + 1, \\ \deg \tilde{p}_{1,i} - \deg p_{n_1+1}^2 &> \deg(p_j \partial_i q_j) - \deg(p_{n_1+1} q_j), & j = n_1 + 2, \dots, n_1 + n_2 + 1, \\ \deg \tilde{p}_{1,i} - \deg p_{n_1+1}^2 &> \deg \partial_i q_{n_1+1} - \deg q_{n_1+1}. \end{aligned}$$

If $j_0 = n_1 + 1$, then we pick up i satisfying $\deg \partial_i q_{n_1+1} \neq -\infty$. It follows that

$$\deg \partial_i q_{n_1+1} - \deg q_{n_1+1} = -1.$$

Consequently,

$$\begin{aligned} \deg \partial_i q_{n_1+1} - \deg q_{n_1+1} &> \deg \tilde{p}_{j,i} - \deg p_{n_1+1}^2, & j = 1, \dots, n_1 + n_2 + 1, \\ \deg \partial_i q_{n_1+1} - \deg q_{n_1+1} &> \deg(p_j \partial_i q_j) - \deg(p_{n_1+1} q_j), & j = n_1 + 2, \dots, n_1 + n_2 + 1. \end{aligned}$$

Thus we conclude from the induction hypothesis that Lemma 2.6 is true when n_2 is replaced by $n_2 + 1$. This completes the proof. \square

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