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A TWO-SCALE HIGHER-ORDER FINITE ELEMENT DISCRETIZATION FOR SCHRÖDINGER EQUATION*

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Abstract

In this paper, a two-scale higher-order finite element discretization scheme is proposed and analyzed for a Schrödinger equation on tensor product domains. With the scheme, the solution of the eigenvalue problem on a fine grid can be reduced to an eigenvalue problem on a much coarser grid together with some eigenvalue problems on partially fine grids. It is shown theoretically and numerically that the proposed two-scale higher-order scheme not only significantly reduces the number of degrees of freedom but also produces very accurate approximations.

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1. Introduction

Theoretical analysis of the electronic structure of matter is usually based on the energy-levels and wavefunctions of the many-body particle system. As a result, a number of eigenvalues and eigenfunctions of the Schrödinger type equations are required to be computed accurately and efficiently. However, it is a challenging task to solve multi-dimensional eigenvalue problems by conventional discretization methods, due to storage requirements and computational complexity.

In order to reduce the computational costs, such as the computational time and the storage requirement, we will introduce a two-scale higher-order finite element discretization scheme to solve the associated eigenvalue problem. With the scheme, the solution of the eigenvalue problem on a fine grid can be reduced to an eigenvalue problem on a much coarser grid and some eigenvalue problems on partially fine grids. It is shown by both theory and numerics that the scheme is efficient. The work of this paper may be viewed as a generalization of that in [14, 21, 22], in which some two-scale linear finite element discretizations for solving partial differential equations in multi-dimensions were developed.

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In the modern electronic structure computation of large scale, the pseudopotential formulations of the Kohn-Sham equations should be used. Note that in the pseudopotentional setting, the associated effective potentials of the Kohn-Sham equations are smooth [4, 5, 23, 24, 27], though the original effective potentials are singular. Hence we may start our investigation from the following Schrödinger equation:

$$\begin{cases} -\frac{1}{2}\Delta u + Vu = \lambda u & \text{in} \quad \Omega, \\ \qquad\qquad u = 0 & \text{on} \quad \partial\Omega, \end{cases} \tag{1.1}$$

where $\Omega = (0,1)^3$ and the effective potential V is smooth, say, $V \in W^{1,\infty}(\Omega)$.

We now give a somewhat more detailed description of the main ideas and results in this paper. Let $S_0^{h_1,h_2,h_3}(\Omega) \subset H_0^1(\Omega)$ be the standard triquadratic finite element space associated with the finite element mesh $T^{h_1,h_2,h_3}(\Omega)$ with mesh size h_1 in x-direction, h_2 in y-direction and h_3 in z-direction, respectively. One prototype scheme to discretize (1.1), say for the first eigenvalue λ with its corresponding eigenfunction u with $\int_\Omega |u|^2 = 1$, is as follows:

1. Solve (1.1) on a globally coarse grid: Find $(u_{H,H,H}, \lambda_{H,H,H}) \in S_0^{H,H,H}(\Omega) \times \mathbb{R}$ such that $\int_\Omega |u_{H,H,H}|^2 = 1$ and

$$\int_\Omega \frac{1}{2}\nabla u_{H,H,H} \cdot \nabla v + V u_{H,H,H} \cdot v = \lambda_{H,H,H} \int_\Omega u_{H,H,H} \cdot v, \quad \forall v \in S_0^{H,H,H}(\Omega).$$

2. Solve (1.1) on some partially fine grids in parallel:
   Find $(u_{h,H,H}, \lambda_{h,H,H}) \in S_0^{h,H,H}(\Omega) \times \mathbb{R}$ such that $\int_\Omega |u_{h,H,H}|^2 = 1$ and

$$\int_\Omega \frac{1}{2}\nabla u_{h,H,H} \cdot \nabla v + V u_{h,H,H} \cdot v = \lambda_{h,H,H} \int_\Omega u_{h,H,H} \cdot v, \quad \forall v \in S_0^{h,H,H}(\Omega);$$

   Find $(u_{H,h,H}, \lambda_{H,h,H}) \in S_0^{H,h,H}(\Omega) \times \mathbb{R}$ such that $\int_\Omega |u_{H,h,H}|^2 = 1$ and

$$\int_\Omega \frac{1}{2}\nabla u_{H,h,H} \cdot \nabla v + V u_{H,h,H} \cdot v = \lambda_{H,h,H} \int_\Omega u_{H,h,H} \cdot v, \quad \forall v \in S_0^{H,h,H}(\Omega);$$

   Find $(u_{H,H,h}, \lambda_{H,H,h}) \in S_0^{H,H,h}(\Omega) \times \mathbb{R}$ such that $\int_\Omega |u_{H,H,h}|^2 = 1$ and

$$\int_\Omega \frac{1}{2}\nabla u_{H,H,h} \cdot \nabla v + V u_{H,H,h} \cdot v = \lambda_{H,H,h} \int_\Omega u_{H,H,h} \cdot v, \quad \forall v \in S_0^{H,H,h}(\Omega).$$

3. Set

$$\begin{aligned} u^h_{H,H,H} &= u_{h,H,H} + u_{H,h,H} + u_{H,H,h} - 2u_{H,H,H}, \\ \lambda^h_{H,H,H} &= \lambda_{h,H,H} + \lambda_{H,h,H} + \lambda_{H,H,h} - 2\lambda_{H,H,H}. \end{aligned}$$

If, for example, $\lambda_{H,H,H}$, $\lambda_{h,H,H}$, $\lambda_{H,h,H}$, and $\lambda_{H,H,h}$ are the first eigenvalues of the corresponding problems, then we can establish the following results (see Theorem 4.1 in Section 4 below)

$$\left(\int_\Omega |u - u^h_{H,H,H}|^2\right)^{1/2} = \mathcal{O}(h^3 + H^5) \text{ and } |\lambda - \lambda^h_{H,H,H}| = \mathcal{O}(h^4 + H^6)$$

provided that u has some reasonable regularity. These estimates mean that we can obtain asymptotically optimal approximation by taking $H = \mathcal{O}(h^{3/5})$ for eigenfunctions, and $H = \mathcal{O}(h^{2/3})$ for eigenvalues. Our technical tools for analyzing two-scale finite element approximations are some superconvergence techniques developed in [14, 20, 26] (see, also, [17–19, 35]).

The remainder of this paper is arranged as follows: In the coming section, some preliminary materials, including two error estimations of finite element interpolants in a weak form, are provided. With the two-scale finite element analysis in Section 3, which is a generalization of [14, 21, 22] to higher-order finite element methods, a two-scale higher-order element scheme is then analyzed for eigenvalue problems in Section 4. In Section 5, several numerical results, which support our theory, are reported. Finally, some remarks are concluded and a generalization for a more general elliptic eigenvalue problem is presented in Appendix.

2. Preliminaries

Let $\Omega = (0,1)^d (d \geq 2)$. We shall use the standard notation for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms and seminorms, see, e.g., [1,10]. For $p = 2$, we denote $H^s(\Omega) = W^{s,2}(\Omega)$ and $H_0^1(\Omega) = \{v \in H^1(\Omega) : v\mid_{\partial\Omega} = 0\}$, where $v\mid_{\partial\Omega} = 0$ is in the sense of trace, $\|\cdot\|_{s,\Omega} = \|\cdot\|_{s,2,\Omega}$ and $\|\cdot\|_{\Omega} = \|\cdot\|_{0,2,\Omega}$. We let $(\cdot,\cdot)$ to be the standard inner-product of $L^2(\Omega)$. Throughout this paper, we shall assume that the effective potential $V \in W^{1,\infty}(\Omega)$. And we use letter C (with or without subscripts) to denote a generic positive constant which may stand for different values at its different occurrences. For convenience, the symbol $\lesssim$ will be used in this paper. The notation that $A \lesssim B$ means that $A \leq CB$ for some constant C that is independent of mesh parameters.

We denote by $\mathbb{N}_0$ the set of all nonnegative integers and $\mathbb{Z}_d = \{1, 2, \cdots, d\}$. For a function $w \in W^{s,p}(\Omega)$, a point $x = (x_1, x_2, \ldots, x_d) \in \Omega$ and the index $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_d) \in \mathbb{N}_0^d$, we let

$$(D^{\boldsymbol{\alpha}} w)(x) = \left(\frac{\partial^{\boldsymbol{\alpha}_1}}{\partial x_1^{\boldsymbol{\alpha}_1}} \cdots \frac{\partial^{\boldsymbol{\alpha}_d} w}{\partial x_d^{\boldsymbol{\alpha}_d}} \right)(x)$$

with $|\boldsymbol{\alpha}| = \alpha_1 + \cdots + \alpha_d$. Furthermore, we denote $\mathbf{0} = (0, \ldots, 0) \in \mathbb{R}^d$, $\mathbf{e} = (1, \ldots, 1) \in \mathbb{R}^d$ and for $i \in \mathbb{Z}_d$, $\hat{\mathbf{e}}_i = \mathbf{e} - \mathbf{e}_i$ and $\mathbf{e}_i = (0, \ldots, 0, 1, 0, \ldots, 0) \in \mathbb{R}^d$ whose ith component is one and zero otherwise.

The following mixed Sobolev spaces, which contain $H^{p+3}(\Omega)$ and $H^{p+2}(\Omega)$ respectively, are also used:

$$\begin{aligned}
W^{G,p+3}(\Omega) &= \big\{ w \in H^{p+2}(\Omega) : \ D^{\boldsymbol{\alpha}} w \in L^2(\Omega), \ \mathbf{0} \leq \boldsymbol{\alpha} \leq (p+2)\mathbf{e}, \ |\boldsymbol{\alpha}| = p+3 \big\}, \\
W^{G,p+2}(\Omega) &= \big\{ w \in H^{p+1}(\Omega) : \ D^{\boldsymbol{\alpha}} w \in L^2(\Omega), \ \mathbf{0} \leq \boldsymbol{\alpha} \leq (p+1)\mathbf{e}, \ |\boldsymbol{\alpha}| = p+2 \big\},
\end{aligned}$$

with their natural norms $\|\cdot\|_{W^{G,p+3}(\Omega)}$ and $\|\cdot\|_{W^{G,p+2}(\Omega)}$ (cf. [26]).

For $t \in (p, p+1)$, we define the fractional mixed Sobolev space $W^{G,t+2}(\Omega)$ by using the interpolation approach (see, e.g., [6]) as follows: Set $\theta = t - p$ and define

$$\begin{aligned}
K(s,u) &= \inf_{v \in W^{G,p+3}(\Omega)} \left(\|u - v\|_{W^{G,p+2}(\Omega)} + s\|v\|_{W^{G,p+3}(\Omega)} \right), \\
W^{G,t+2}(\Omega) &\equiv \big[W^{G,p+2}(\Omega), W^{G,p+3}(\Omega) \big]_\theta \\
&= \big\{ u \in W^{G,p+2}(\Omega) : \|u\|_{[W^{G,p+2}(\Omega), W^{G,p+3}(\Omega)]_\theta} < \infty \big\},
\end{aligned} \tag{2.1}$$

where

$$\|u\|_{[W^{G,p+2}(\Omega),W^{G,p+3}(\Omega)]_\theta} = \left(\int_0^\infty s^{-2\theta-1}[K(s,u)]^2 ds\right)^{1/2}.$$

Let $T^h(\Omega)$ consist of $d-$rectangles, which satisfies that it is not exceedingly over-refined locally, namely, there exists $\gamma \geq 1$ such that

$$h^\gamma \lesssim h(x), \quad \forall x \in \Omega, \tag{2.2}$$

where $h(x)$ is the mesh-size function whose value is the diameter h_τ of the element τ containing x, $h = \max_{x\in\Omega} h(x)$ is the (largest) mesh size of $T^h(\Omega)$. Define $S^{h,p}(\Omega)$ to be a space of continuous piecewise polynomial on Ω:

$$S^{h,p}(\Omega) = \{v \in C(\bar{\Omega}) : v\mid_\tau \in Q_p(\tau), \quad \forall \tau \in T^h(\Omega)\}, \tag{2.3}$$

where $Q_p(\tau)$ is the space of all polynomials that are of degree not greater than p with respect to each of the d variables. Set

$$S_0^{h,p}(\Omega) = H_0^1(\Omega) \cap S^{h,p}(\Omega).$$

To obtain the error estimates of the finite element approximation, we need some regularity information of the Schrödinger equation (see, e.g., [12]):

Proposition 2.1. *Assume that $f \in H^s(\Omega)$ for some $s \geq 0$ and*

$$\begin{cases} -\frac{1}{2}\Delta u + Vu = f & in \quad \Omega, \\ u = 0 & on \quad \partial\Omega \end{cases} \tag{2.4}$$

has a unique solution $u \in H_0^1(\Omega)$. Then $u \in H_0^1(\Omega) \cap H^{s+2}(\Omega)$ for $s \in [0,1)$. Moreover, if $f = 0$ at corners (when $d = 2$), and along edges (when $d = 3$, and with the appropriate definition of edges when $d \geq 4$), then $u \in H_0^1(\Omega) \cap H^{s+2}(\Omega)$ and

$$\|u\|_{s+2,\Omega} \lesssim \|f\|_{s,\Omega} \tag{2.5}$$

for all $s \in [0,3)$.

2.1. An Eigenvalue Problem

Define

$$a(u,v) = \int_\Omega \frac{1}{2}\nabla u \nabla v + Vuv, \quad u,v \in H_0^1(\Omega). \tag{2.6}$$

A number λ is called an eigenvalue of $a(\cdot,\cdot)$ relative to $(\cdot,\cdot)$ if there is a nonzero vector $u \in H_0^1(\Omega)$, called an associated eigenfunction, satisfying

$$a(u,v) = \lambda(u,v), \quad \forall v \in H_0^1(\Omega). \tag{2.7}$$

It is easy to obtain from (2.6) and $V \in W^{1,\infty}(\Omega)$ that there exist $\nu \geq 0$, such that

$$a_\nu(w,w) \geq C^{-1}\|w\|^2, \quad \forall w \in H_0^1(\Omega) \tag{2.8}$$

for some constant C, where

$$a_\nu(w,v) = a(w,v) + \nu(u,v), \quad w,v \in H_0^1(\Omega). \tag{2.9}$$

Note that (2.7) is equivalent to

$$a_\nu(u,v) = E(u,v), \quad \forall v \in H_0^1(\Omega)$$

with $E = \lambda + \nu$. Hence (2.7) has a countable sequence of real eigenvalues

$$\lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots$$

and the corresponding eigenfunctions

$$u_1, u_2, u_3, \cdots,$$

which can be assumed to satisfy

$$(u_i, u_j) = \delta_{ij}, \quad i,j = 1,2,\cdots.$$

In the sequence $\{\lambda_j\}$, the λ_j's are repeated according to their geometric multiplicity.

A standard finite element scheme for (2.7) is: Find a pair of (λ_h, u_h), where $\lambda_h \in \mathbb{R}$ and $0 \ne u_h \in S_0^{h,p}(\Omega)$, satisfying

$$a(u_h, v) = \lambda_h(u_h, v), \quad \forall v \in S_0^{h,p}(\Omega), \tag{2.10}$$

or

$$a_\nu(u_h, v) = E_h(u_h, v), \quad \forall v \in S_0^{h,p}(\Omega) \tag{2.11}$$

with $E_h = \lambda_h + \nu$. One sees from (2.8) that (2.10) has a finite sequence of eigenvalues

$$\lambda_{1,h} \le \lambda_{2,h} \le \cdots \le \lambda_{n_h,h}, \quad n_h = \dim S_0^{h,p}(\Omega)$$

and the corresponding eigenfunctions

$$u_{1,h}, u_{2,h}, \cdots, u_{n_h,h},$$

which can be assumed to satisfy

$$(u_{i,h}, u_{j,h}) = \delta_{ij}, \ i,j = 1,2,\cdots.$$

It follows directly from the minimum-maximum principle (see, e.g., [3]) that

$$\lambda_i \le \lambda_{i,h}, \quad i = 1,2,\cdots,n_h.$$

Set

$$\begin{aligned} M(\lambda_i) &= \big\{w \in H_0^1(\Omega) : w \text{ is an eigenfunction of (2.7) corresponding to } \lambda_i\big\}, \\ \delta_h(\lambda_i) &= \sup_{w \in M(\lambda_i), \|w\|_{0,\Omega}=1} \inf_{v \in S_0^h(\Omega)} \|w - v\|_{1,\Omega}. \end{aligned}$$

The following results are standard and can be found in the literature (see, e.g., [2, 3, 9] or [32]).

Proposition 2.2. *(i) For any $u_{i,h}$ of* (2.10) *with $\|u_{i,h}\|_{0,\Omega} = 1$, there is an eigenfunction u^i of* (2.7) *corresponding to λ_i satisfying $\|u^i\|_{0,\Omega} = 1$ and*

$$\|u^i - u_{i,h}\|_{1,\Omega} \le C_i \delta_h(\lambda_i). \tag{2.12}$$

Moreover,

$$\|u^i - u_{i,h}\|_{0,\Omega} \le C_i h \|u^i - u_{i,h}\|_{1,\Omega}. \tag{2.13}$$

(ii) For eigenvalues,

$$\lambda_i \le \lambda_{i,h} \le \lambda_i + C_i \|u^i - u_{i,h}\|_{1,\Omega}^2, \quad i = 1, 2, \cdots. \tag{2.14}$$

Here C_i is some positive constant depending on i but not on the mesh parameter h.

The two-scale analysis for the eigenvalues is based on the following crucial (but straightforward) property of eigenvalue and eigenfunction approximation (see [3, 32]).

Proposition 2.3. *Let (λ, u) be an eigenpair of* (2.7). *For any $w \in H_0^1(\Omega) \setminus \{0\}$,*

$$\frac{a(w,w)}{(w,w)} - \lambda = \frac{a(w-u, w-u)}{(w,w)} - \lambda \frac{(w-u, w-u)}{(w,w)}. \tag{2.15}$$

2.2. Some Basic Analysis

For simplicity, we may assume that $\nu = 0$ in (2.9). Consequently, (2.4) is uniquely solvable for any $f \in L^2(\Omega)$. Define a Galerkin projection $P_h : H_0^1(\Omega) \to S_0^{h,p}(\Omega)$ by

$$a(w - P_h w, v) = 0, \quad \forall v \in S_0^{h,p}(\Omega), \tag{2.16}$$

for which there holds

$$\|P_h w\|_{1,\Omega} \lesssim \|w\|_{1,\Omega}, \quad \forall w \in H_0^1(\Omega). \tag{2.17}$$

Then various a priori global error estimates can be obtained from the approximate properties of the finite element space $S^{h,p}(\Omega)$. For instance, if $w \in H_0^1(\Omega) \cap H^{t+1}(\Omega) (t \in [0,p])$ holds, then (see, e.g., [6, 10])

$$\|(I - P_h) w\|_{1,\Omega} \lesssim h^t \|w\|_{t+1,\Omega}, \tag{2.18}$$

$$\|(I - P_h) w\|_{0,\Omega} \lesssim h \|(I - P_h) w\|_{1,\Omega}, \quad \forall w \in H_0^1(\Omega), \tag{2.19}$$

where I is the identity operator.

There is some superclose relationship between the Galerkin projection of the eigenfunction and the finite element approximation to the eigenfunction, which can be deduced from [32]:

Proposition 2.4. *Let $u_{i,h}$ be a solution of* (2.10), *and $P_h u^i$ be the Ritz-Galerkin projection of u^i, then we have*

$$\|P_h u^i - u_{i,h}\|_{1,\Omega} \lesssim \lambda_{i,h} - \lambda_i + \lambda_i \|u^i - u_{i,h}\|_{0,\Omega}. \tag{2.20}$$

Define a linear operator $K : L^2(\Omega) \to H_0^1(\Omega)$ by

$$a(Kw, v) = (w, v), \quad \forall w \in L^2(\Omega), \quad \forall v \in H_0^1(\Omega). \tag{2.21}$$

Then (2.7) becomes

$$u = \lambda K u \tag{2.22}$$

and (2.10) can be rewritten as

$$u_h = \lambda_h P_h K u_h. \tag{2.23}$$

It is derived from Proposition 2.1 that

$$M(\lambda_i) \subset H^{s+1}(\Omega) \subset W^{G,s+1}(\Omega), \quad \forall s \in [0, 4) \tag{2.24}$$

and hence

$$\|u\|_{s+1,\Omega} \lesssim \|u\|_{0,\Omega} \tag{2.25}$$

for $u \in M(\lambda_i)$.

In the remainder of this subsection, for simplicity, we assume that $(\lambda_h, u_h) \in \mathbb{R} \times S_0^{h,p}(\Omega)$ is some finite element eigenpair of (2.10) with $\|u_h\|_{0,\Omega} = 1$ while $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$ is the associated exact eigenpair of (2.7) that satisfies $\|u\|_{0,\Omega} = 1$ and

$$\|u - u_h\|_{0,\Omega} + |\lambda - \lambda_h| \le C\big(h + \|u - u_h\|_{1,\Omega}\big)\|u - u_h\|_{1,\Omega}. \tag{2.26}$$

Consequently, if $M(\lambda_i) \subset H^{t+1}(\Omega)\big(t \in [0, p]\big)$, then

$$|\lambda_h - \lambda| \lesssim h^{2t}, \tag{2.27}$$

$$\|u - u_h\|_{0,\Omega} + h\|u - u_h\|_{1,\Omega} \lesssim h^{t+1}, \tag{2.28}$$

which leads to

$$\Big\| \frac{\lambda_h - \lambda}{\lambda}(u - P_h u) + (\lambda - \lambda_h)K(u - u_h) \Big\|_{1,\Omega} \lesssim h^{3t}, \tag{2.29}$$

$$\Big\| \frac{\lambda_h - \lambda}{\lambda}(u - P_h u) + (\lambda - \lambda_h)K(u - u_h) \Big\|_{0,\Omega} \lesssim h^{3t+1}. \tag{2.30}$$

Lemma 2.1. *If $M(\lambda) \subset H^{t+1}(\Omega)\big(t \in [0, p]\big)$, then*

$$\lambda_h - \lambda = \lambda(u, u - P_h u) + \mathcal{O}\big(h^{2t+2}\big). \tag{2.31}$$

Proof. It is obtained from (2.7) and (2.10) that (see [14] for details)

$$\begin{aligned} \lambda_h - \lambda =& \lambda(u, u - P_h u) + (\lambda_h - \lambda)(u_h, u_h - P_h u) \\ &+ \lambda(u_h - u, u_h - P_h u) - \lambda\|u - u_h\|_{0,\Omega}^2, \end{aligned}$$

which, together with (2.27), (2.28) and (2.20) produces (2.31). This completes the proof. □

Lemma 2.2. *There holds*

$$(I-\lambda K)(u-u_h)=\frac{1}{\lambda}(\lambda-\lambda_h)u+u-P_hu+r_h(u), \tag{2.32}$$

where

$$r_h(u)=\frac{\lambda_h-\lambda}{\lambda}(u-P_hu)+(\lambda_h-\lambda)K(u-u_h)+\lambda_h(P_h-I)K(u-u_h)$$

satisfying

$$\|r_h(u)\|_{0,\Omega}+h\|r_h(u)\|_{1,\Omega}\lesssim h^{2t+2} \tag{2.33}$$

provided that $M(\lambda)\subset H^{t+1}(\Omega)\big(t\in[0,p]\big)$.

Proof. The identity (2.32) can be established by using (2.22) and (2.23) (see [14] for details). Since (2.18), (2.19) and (2.25) imply that

$$\begin{aligned}
&\|(P_h-I)K(u-u_h)\|_{0,\Omega}+h\|(P_h-I)K(u-u_h)\|_{1,\Omega}\\
\lesssim& h^{t+1}\|K(u-u_h)\|_{t+1,\Omega}\lesssim h^{t+1}\|u-u_h\|_{0,\Omega}\\
\lesssim& h^{2t+2}\|u\|_{t+1,\Omega},
\end{aligned}$$

we can derive (2.33) from (2.27)-(2.30). This completes the proof. $\square$

2.3. Finite element interpolants

To generalize the two-scale discretization approach in [21,22] to higher-order finite element in arbitrary dimensions, we need to apply the superconvergence techniques developed in [14,17, 18,21,22,26,35], which concern some error estimations of finite element interpolants in a weak form setting.

Assume that $T^h\big((0,1)\big)$ is a uniform mesh with mesh size h on $(0,1)$ and $S^{h,p}\big((0,1)\big)\subset H^1\big((0,1)\big)$ $(p\ge 2)$ is the associated piecewise higher-order finite element space. Set

$$S_0^{h,p}\big((0,1)\big)=S^{h,p}\big((0,1)\big)\cap H_0^1\big((0,1)\big).$$

We next describe the multi-dimensional notation. For $\mathbf{h}=(h_1,\dots,h_d)$, where $h_j\in(0,1)$, construct a mesh of $\Omega=(0,1)^d$ by

$$T^{\mathbf{h}}(\Omega)=T^{h_1}\big((0,1)\big)\times\cdots\times T^{h_d}\big((0,1)\big)$$

with the associated spaces of piecewise polynomials on Ω by

$$\begin{aligned}
S^{\mathbf{h},p}(\Omega)&=S^{h_1,p}\big((0,1)\big)\otimes\cdots\otimes S^{h_d,p}\big((0,1)\big),\\
S_0^{\mathbf{h},p}(\Omega)&=S_0^{h_1,p}\big((0,1)\big)\otimes\cdots\otimes S_0^{h_d,p}\big((0,1)\big).
\end{aligned}$$

We remark that both $S^{\mathbf{h},p}(\Omega)$ and $S_0^{\mathbf{h},p}(\Omega)$ are the tensor product spaces of the spaces of piecewise polynomials of degree not greater than p on $(0,1)$.

Instead of the standard Lagrangian interpolation, in our analysis, we need to use a so-called "vertices-edges-area" interpolation [15,20,35]. For $l\in\mathbb{Z}_d$, let $I_{h_l}:C\big([0,1]\big)\to S^{h_l,p}\big([0,1]\big)$ be defined by: For all $\big(x_l^i,x_l^{i+1}\big)\in T^{h_l}\big((0,1)\big)$

$$\begin{aligned}
&I_{h_l}u(x_l^i)=u(x_l^i),\quad I_{h_l}u(x_l^{i+1})=u(x_l^{i+1}),\\
&\int_{x_l^i}^{x_l^{i+1}}(u-I_{h_l}u)v\,dx_l=0,\quad\forall v\in P_{p-2}(x_l^i,x_l^{i+1}),
\end{aligned} \tag{2.34}$$

where $P_p(\tau)$ denotes the set of polynomials of degree not greater than p on τ. It is shown that (see, e.g., [15, 20, 35])

$$\begin{aligned}
&I_{h_l}v = v, \quad \forall v \in S^{h_l,p}([0,1]),\\
&\|I_{h_l}v\|_{s,[0,1]} \le C\|v\|_{s,[0,1]}, \quad \forall v \in C([0,1]),\ s=0,1,\\
&\|v - I_{h_l}v\|_{0,[0,1]} + h_l\|v - I_{h_l}v\|_{1,[0,1]}\\
\le& Ch_l^{t+1}\|v\|_{t+1,\Omega}, \quad \forall v \in C([0,1]),\ t \in [0,p].
\end{aligned} \tag{2.35}$$

The so-called interpolation "vertices-edges-area" operator $I_{\mathbf{h},p}$ from $C(\overline{\Omega})$ onto $S^{\mathbf{h}}(\overline{\Omega})$ is constructed as $I_{\mathbf{h}} = I_{h_1} \circ \cdots \circ I_{h_d}$. For $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_d) \in \mathbb{N}_0^d$, we set

$$\mathbf{h}^{\boldsymbol{\alpha}} = h_1^{\alpha_1} \cdots h_d^{\alpha_d}, \quad \mathbf{h}\boldsymbol{\alpha} = (h_1\alpha_1, \ldots, h_d\alpha_d).$$

From the standard interpolation error estimation, we immediately obtain

Proposition 2.5. *Assume that $w \in H_0^1(\Omega) \cap W^{G,t+2}(\Omega)$ $(t \in [p, p+1])$. If $\mathbf{0} \le \boldsymbol{\alpha} \le \mathbf{e}$ and $|\boldsymbol{\alpha}| \ge 2$, then*

$$\begin{aligned}
&a\bigg(\prod_{0\le\boldsymbol{\beta}\le\boldsymbol{\alpha},|\boldsymbol{\beta}|=1}\big(I - I_{\mathbf{h}\boldsymbol{\beta}}\big)w, v\bigg)\\
\lesssim& \max_{\mathbf{0}\le\boldsymbol{\mu}\le p\mathbf{e},\ |\boldsymbol{\mu}|=t+1} \mathbf{h}^{\boldsymbol{\mu}}\|w\|_{W^{G,t+2}(\Omega)}\|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega),
\end{aligned} \tag{2.36}$$

where $a(\cdot,\cdot)$ is defined by (2.6).

The following result may be viewed as a generalization of the relevant result known in the literature (see, e.g., [17–20, 35, 36]). Novelties of our estimate lie in, for example, the weak assumption on the regularity of the function. Although the general estimate is theoretically interesting, our main motivation is to use it to analyze some two-scale finite element discretizations to be presented in the coming sections.

Proposition 2.6. *If $w \in H_0^1(\Omega) \cap W^{G,t+2}(\Omega)$ $\big(t \in [p, p+1]\big)$, then*

$$a\big((I - I_{\mathbf{h}})w, v\big) \lesssim \max_{|\boldsymbol{\alpha}|=t+1} \mathbf{h}^{\boldsymbol{\alpha}}\|w\|_{W^{G,t+2}(\Omega)}\|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \tag{2.37}$$

Proof. The estimation for $t = p$ is referred to the Appendix (see Proposition A.1), and it is only necessary to give the proof for $t = p+1$ by using the interpolation theory (see, e.g., [6, 10, 28, 29]). For simplicity, we denote $\frac{\partial^l}{\partial^l_{x_i}}$ by $\partial^l_{x_i}(i \in \mathbb{Z}_d, l \in \mathbb{N}_0)$.

First, using the fact that $\partial^2_{x_l}v$ is a polynomial of degree not greater than $p-2$ with respect to the variable x_l and integrating by parts lead to

$$\int_\tau \partial_{x_l}\big(I - I_{\mathbf{h}\mathbf{e}_l}\big)w\partial_{x_l}v = 0, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \tag{2.38}$$

Now for $i \ne l$ and $l \in \mathbb{Z}_d$, we define $F_l : \bar{\Omega} \to \mathbb{R}$ by

$$F_l(\mathbf{x}) = \frac{1}{2}\left((x_l - x_{\tau,l})^2 - \frac{h_l^2}{4}\right) \quad \text{if } x \in \bar{\tau} \in T^{\mathbf{h}}(\Omega), \tag{2.39}$$

where $x_\tau = (x_{\tau,1}, x_{\tau,2}, \cdots, x_{\tau,d})$ is the barycenter of τ and $x = (x_1, x_2, \cdots, x_d) \in \Omega$. By simple calculation using Leibniz derivation rule, it is easy to see that $F_l \in C(\bar{\Omega})$ and for $m = 2, 3, \cdots, p$, there is a polynomial $R_m(x_l) \in P_{m-2} \subset P_{p-2}$ such that (cf. [35])

$$\frac{1}{m!}(x_l - x_{\tau,l})^m = \frac{2^{m+1}}{(2m+2)!}\big(F_l^{m+1}(x_l)\big)^{(m+2)} + R_m(x_l), \tag{2.40}$$

$$\big(F_l^{m+1}(x_{\tau,l} \pm \frac{h_l}{2})\big)^{(n)} = 0 \quad \text{for } n \le m. \tag{2.41}$$

So using Taylor's expansion, we have for $v \in S_0^{\mathbf{h},p}(\Omega)$ that

$$\int_\tau \partial_{x_i}(I - I_{\mathbf{he}_l})w\partial_{x_i}v = \int_\tau (I - I_{\mathbf{he}_l})\partial_{x_i}w\Big(\sum_{j=0}^{p}\frac{1}{j!}\big(x_l - x_{\tau,l}\big)^j\partial_{x_i}\partial_{x_l}^j v\big(x_{\tau,l}\big)\Big).$$

Note that for $j \le p-2$,

$$\int_\tau (I - I_{\mathbf{he}_l})\partial_{x_i}w\Big(\sum_{j=0}^{p-2}\frac{1}{j!}(x_l - x_{\tau,l})^j\partial_{x_i}\partial_{x_l}^j v(x_{\tau,l})\Big) = 0,$$

where (2.34) is used. Integrating by parts, we then obtain for $j = p-1$ and $j = p$ respectively that

$$\begin{aligned}
&\int_\tau (I - I_{\mathbf{he}_l})\partial_{x_i}w\frac{1}{j!}\big(x_l - x_{\tau,l}\big)^j\partial_{x_i}\partial_{x_l}^j v(x_{\tau,l}) \\
=&\int_\tau \frac{2^{j+1}}{(2j+2)!}\big(F_l^{j+1}(x_l)\big)^{(j+2)}\big(I - I_{\mathbf{he}_l}\big)\partial_{x_i}w\partial_{x_i}\partial_{x_l}^j v\big(x_{\tau,l}\big) \\
&+ R_j(x_l)\big(I - I_{\mathbf{he}_l}\big)\partial_{x_i}w\partial_{x_i}\partial_{x_l}^j v\big(x_{\tau,l}\big) \\
=&(-1)^j\int_\tau \frac{2^{j+1}}{(2j+2)!}F_l^{j+1}(x_l)\partial_{x_l}^{j+2}\big(I - I_{\mathbf{he}_l}\big)\partial_{x_i}w\partial_{x_i}\partial_{x_l}^j v\big(x_{\tau,l}\big) \\
=&\frac{(-1)^j 2^{j+1}}{(2j+2)!}\int_\tau F_l^{j+1}(x_l)\partial_{x_l}^{j+2}\partial_{x_i}w\partial_{x_i}\partial_{x_l}^j v\big(x_{\tau,l}\big).
\end{aligned}$$

Taking the three parts above into account, we arrive at

$$\begin{aligned}
&\int_\Omega \partial_{x_i}\big(I - I_{\mathbf{he}_l}\big)w\partial_{x_i}v \\
=&\sum_{\tau\in T^{\mathbf{h}}(\Omega)}\Big(\frac{(-1)^{p+1}2^p}{(2p)!}\int_\tau F_l^p(x_l)\partial_{x_l}^{p+1}\partial_{x_i}^2 w\partial_{x_l}^{p-1}v\big(x_{\tau,l}\big) \\
&+\frac{(-1)^p 2^{p+1}}{(2p+2)!}\int_\tau F_l^{p+1}(x_l)\partial_{x_l}^{p+2}\partial_{x_i}w\partial_{x_i}\partial_{x_l}^p v\big(x_{\tau,l}\big)\Big) \\
\lesssim&\, h_l^{p+2}\|w\|_{W^{G,p+3}(\Omega)}\|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega),
\end{aligned} \tag{2.42}$$

where integration by parts and the inverse estimate are employed. Using the error estimate

$$\|Vv - V(x_\tau)v(x_\tau)\|_{0,\tau} \lesssim h_l\|V\|_{1,\infty,\tau}\|v\|_{1,\tau}, \quad \forall \tau \in T^{\mathbf{h}}(\Omega), l \in \mathbb{Z}_d, v \in S_0^{\mathbf{h},p}(\Omega)$$

and the identity

$$\begin{aligned}
&\int_\Omega V(I - I_{\mathbf{he}_l})wv \\
=&\sum_{\tau\in T^{\mathbf{h}}(\Omega)}\Big(\int_\tau V(x_\tau)v(x_\tau)\big(I - I_{\mathbf{he}_l}\big)w + \int_\tau \Big(Vv - V(x_\tau)v(x_\tau)\Big)\big(I - I_{\mathbf{he}_l}\big)w\Big),
\end{aligned}$$

we obtain

$$\int_\Omega V\big(I - I_{\mathbf{h}\mathbf{e}_l}\big)wv \lesssim h_l^{p+2}\|w\|_{p+1,\Omega}\|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \tag{2.43}$$

Obviously, for any $v \in S_0^{\mathbf{h},p}(\Omega)$ and $l \in \mathbb{Z}_d$,

$$\begin{aligned} &a\big((I - I_{\mathbf{h}\mathbf{e}_l})w, v\big) \\ &= \int_\Omega \partial_{x_l}\big(I - I_{\mathbf{h}\mathbf{e}_l}\big)w\partial_{x_l}v + \sum_{i=1, i\neq l}^{d}\int_\Omega \partial_{x_i}\big(I - I_{\mathbf{h}\mathbf{e}_l}\big)w\partial_{x_i}v + \int_\Omega V\big(I - I_{\mathbf{h}\mathbf{e}_l}\big)wv. \end{aligned}$$

Thus we get from (2.38), (2.42), (2.43) and the standard interpolation error estimation that

$$a\big((I - I_{\mathbf{h}\mathbf{e}_l})w, v\big) \lesssim h_l^{p+2}\|w\|_{W^{G,p+3}(\Omega)}\|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \tag{2.44}$$

Finally, from the identity

$$I - I_{\mathbf{h}} = -\sum_{0\le\boldsymbol{\alpha}\le\mathbf{e}, |\boldsymbol{\alpha}|\ge 1}(-1)^{|\boldsymbol{\alpha}|}\prod_{0\le\boldsymbol{\beta}\le\boldsymbol{\alpha}, |\boldsymbol{\beta}|=1}(I - I_{\mathbf{h}\boldsymbol{\beta}}),$$

we conclude for any $v \in S_0^{\mathbf{h},p}(\Omega)$ that

$$\begin{aligned} &a\big((I - I_{\mathbf{h}})w, v\big) \\ &= \sum_{0\le\boldsymbol{\alpha}\le\mathbf{e}, |\boldsymbol{\alpha}|=1} a\big((I - I_{\mathbf{h}\boldsymbol{\alpha}})w, v\big) - \sum_{0\le\boldsymbol{\alpha}\le\mathbf{e}, |\boldsymbol{\alpha}|\ge 2}(-1)^{|\boldsymbol{\alpha}|}a\bigg(\prod_{0\le\boldsymbol{\beta}\le\boldsymbol{\alpha}, |\boldsymbol{\beta}|=1}(I - I_{\mathbf{h}\boldsymbol{\beta}})w, v\bigg). \end{aligned}$$

Therefore we derive (2.37) for $t = p+1$ from (2.36), (2.44) and the above result. This completes the proof. □

3. Two-scale Finite Element Analysis

In this section, we will combine the two-scale techniques in [21,22] with higher-order element methods, which may be viewed as a generalization of [14] to higher-order elements. The notation in [14, 21] will be used in our discussion.

3.1. Two-scale finite element interpolants

Given $\sigma \in (0,1)$. Let $w_{\mathbf{h}\boldsymbol{\alpha}+\sigma\boldsymbol{\beta}} \in S^{\mathbf{h}\boldsymbol{\alpha}+\sigma\boldsymbol{\beta},p}(\Omega)$ $\big(\mathbf{0} \le \boldsymbol{\alpha}, \boldsymbol{\beta} \le \mathbf{e}$ and $\boldsymbol{\alpha}+\boldsymbol{\beta} = \mathbf{e}\big)$, and set

$$\delta_\sigma^{\boldsymbol{\alpha}}w_{\mathbf{h}} = \prod_{\alpha_i\neq 0}\delta_\sigma^{\mathbf{e}_i}w_{\mathbf{h}},$$

where $\delta_\sigma^{\mathbf{e}_i}w_{\mathbf{h}} = w_{\mathbf{h}} - w_{\mathbf{h}\hat{\mathbf{e}}_i+\sigma\mathbf{e}_i}$, $i \in \mathbb{Z}_d$. If $d = 2$ and $\mathbf{h} = (h_1, h_2)$, for instance, then

$$\begin{aligned} \delta_\sigma^{(1,0)}w_{h_1,h_2} &= w_{h_1,h_2} - w_{\sigma,h_2}, \\ \delta_\sigma^{(1,1)}w_{h_1,h_2} &= w_{h_1,h_2} - w_{h_1,\sigma} - w_{\sigma,h_2} + w_{\sigma,\sigma}. \end{aligned}$$

Given $h, H \in (0,1)$. Let $w_{H\mathbf{e}} \in S^{H\mathbf{e},p}(\Omega), w_{h\mathbf{e}} \in S^{h\mathbf{e},p}(\Omega)$ and $w_{h\boldsymbol{\alpha}+H\boldsymbol{\beta}} \in S^{h\boldsymbol{\alpha}+H\boldsymbol{\beta},p}(\Omega)$ $\big(\mathbf{0} \le \boldsymbol{\alpha}, \boldsymbol{\beta} \le \mathbf{e}, \boldsymbol{\alpha}+\boldsymbol{\beta} = \mathbf{e}\big)$, and define

$$B_H^h w_{h\mathbf{e}} = w_{H\mathbf{e}} - \sum_{i=1}^{d}\delta_h^{\mathbf{e}_i}w_{H\mathbf{e}}. \tag{3.1}$$

It is shown in the following proposition that a one-scale interpolation on a fine grid can be obtained by some combination of two-scale interpolations asymptotically, which can be derived from the standard one-scale interpolation error estimations (cf. [16, 21, 22] for two- and three-dimensions and [14] for arbitrary dimensions).

Proposition 3.1. *If $t \in [p, p+1]$, then*

$$\begin{aligned} &\|B_H^h I_{h\mathbf{e}} w - I_{h\mathbf{e}} w\|_{0,\Omega} + H\|B_H^h I_{h\mathbf{e}} w - I_{h\mathbf{e}} w\|_{1,\Omega} \\ &\lesssim H^{t+2}\|w\|_{W^{G,t+2}(\Omega)} \quad \text{if } w \in W^{G,t+2}(\Omega). \end{aligned} \tag{3.2}$$

Proof. For $w_{\mathbf{k}} = I_{\mathbf{k}} w$, when $\mathbf{k} = (k_1, k_2, \cdots, k_d)$, we have

$$w_{h\mathbf{e}} = w_{H\mathbf{e}} + \sum_{|\boldsymbol{\alpha}|=1}^{d} (-1)^{|\boldsymbol{\alpha}|} \delta_h^{\boldsymbol{\alpha}} w_{H\mathbf{e}}.$$

Thus we obtain

$$B_H^h w_{h\mathbf{e}} - w_{h\mathbf{e}} = -\sum_{|\boldsymbol{\alpha}|=2}^{d} (-1)^{|\boldsymbol{\alpha}|} \delta_h^{\boldsymbol{\alpha}} w_{H\mathbf{e}}, \tag{3.3}$$

which, together with the standard interpolation error estimations and the interpolation theory (see, e.g., [6, 28, 29]), completes the proof. $\square$

3.2. Two-scale finite element Galerkin projections

Recall that the standard Galerkin projection $P_{\mathbf{h}} : H_0^1(\Omega) \to S_0^{\mathbf{h},p}(\Omega)$ is defined by

$$a(u - P_{\mathbf{h}} u, v) = 0, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega), \tag{3.4}$$

which is well-posed when $\max\{h_i : i \in \mathbb{Z}_d\} \ll 1$ (cf. [30,31]). Here and hereafter, we assume that any mesh size involved is small enough so that the associated discrete problem is well-posed.

Following the two-scale finite element interpolants, we construct the two-scale finite element Galerkin projection as follows:

$$B_{H\mathbf{e}}^h P_{h\mathbf{e}} u = \sum_{i=1}^{d} P_{H\hat{\mathbf{e}}_i + h\mathbf{e}_i} u - (d-1) P_{H\mathbf{e}} u.$$

For instance,

$$B_{H,H,H}^h P_{h,h,h} u = P_{h,H,H} u + P_{H,h,H} u + P_{H,H,h} u - 2P_{H,H,H} u.$$

Theorem 3.1. *If $u \in H_0^1(\Omega) \cap W^{G,t+2}(\Omega)$ $(t \in [p, p+1])$, then*

$$\|B_{H\mathbf{e}}^h P_{h\mathbf{e}} u - P_{h\mathbf{e}} u\|_{0,\Omega} + H\|B_{H\mathbf{e}}^h P_{h\mathbf{e}} u - P_{h\mathbf{e}} u\|_{1,\Omega} \lesssim H^{t+2}\|u\|_{W^{G,t+2}(\Omega)}. \tag{3.5}$$

Moreover,

$$\|B_{H\mathbf{e}}^h P_{h\mathbf{e}} u - P_{h\mathbf{e}} u\|_{1-p,\Omega} \lesssim H^{t+p+1}\|u\|_{W^{G,t+2}(\Omega)} \tag{3.6}$$

holds for $p = 2, 3$.

Proof. The estimation for $t = p$ is referred to the Appendix and we will only need to give the proof for $t = p+1$ by using the interpolation theory (see, e.g., [6, 28, 29]).

Let $\mathbf{h} \in \{H, h\}^d$. It is seen from (2.37) that

$$\|P_{\mathbf{h}}u - I_{\mathbf{h}}u\|_{1,\Omega} \lesssim \max_{i\in\mathbb{Z}_d} \mathbf{h}^{(p+2)\mathbf{e}_i}. \tag{3.7}$$

Hence from the fact

$$\|B^h_{H\mathbf{e}}(P_{h\mathbf{e}} - I_{h\mathbf{e}})u\|_{1,\Omega} \lesssim \max_{\mathbf{h}\in\{H,h\}^d} \|(P_{\mathbf{h}} - I_{\mathbf{h}})u\|_{1,\Omega} \tag{3.8}$$

and the identity

$$B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u = B^h_{H\mathbf{e}}(P_{h\mathbf{e}} - I_{h\mathbf{e}})u + (B^h_{H\mathbf{e}}I_{h\mathbf{e}} - I_{h\mathbf{e}})u + (I_{h\mathbf{e}} - P_{h\mathbf{e}})u, \tag{3.9}$$

we obtain the error estimate under H^1-norm in (3.5) from (3.7) and (3.2).

Now we are going to derive the error estimation under L^2-norm by using the Aubin-Nitsche duality argument. For any $\phi \in L^2(\Omega)$, let $w = (L^*)^{-1}\phi \in H^1_0(\Omega) \cap H^2(\Omega)$. Then

$$\|w - I_{H\mathbf{e}}w\|_{1,\Omega} \lesssim H\|w\|_{2,\Omega} \lesssim H\|\phi\|_{0,\Omega}.$$

Note that

$$\begin{aligned}
&|(B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u, \phi)| = |a(B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u, w)| \\
=&|a(B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u, w - I_{H\mathbf{e}}w)| \lesssim \|B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u\|_{1,\Omega}\|w - I_{H\mathbf{e}}w\|_{1,\Omega},
\end{aligned} \tag{3.10}$$

we obtain

$$|(B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u, \phi)| \lesssim H\|B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u\|_{1,\Omega}\|\phi\|_{0,\Omega},$$

which together with (3.5) implies

$$\|B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u\|_{0,\Omega} \lesssim H^{p+3}\|u\|_{W^{G,p+3}(\Omega)}. \tag{3.11}$$

For the negative norm estimate, let $\phi \in H^{p-1}_0(\Omega)$ and we have from (2.5) that $w = (L^*)^{-1}\phi \in H^1_0(\Omega) \cap H^{p+1}(\Omega)$ and

$$\|w - I_{H\mathbf{e}}w\|_{1,\Omega} \lesssim H^p\|w\|_{p+1,\Omega} \lesssim H^p\|\phi\|_{p-1,\Omega}$$

for $p = 2, 3$. Thus we get from (3.10) and the H^1-norm estimation that

$$|(B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u, \phi)| \lesssim H^p\|B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u\|_{1,\Omega}\|\phi\|_{p-1,\Omega},$$

which together with (3.5) implies

$$\|B^h_{H\mathbf{e}}P_{h\mathbf{e}}u - P_{h\mathbf{e}}u\|_{1-p,\Omega} \lesssim H^{2p+2}\|u\|_{W^{G,p+3}(\Omega)}. \tag{3.12}$$

This completes the proof. $\square$

4. Two-scale Finite Element Eigenvalue Discretizations

In this section, we shall apply the two-scale higher-order finite element methods to solve eigenvalue problems on tensor product grids (see, e.g., [14,21,22]). For simplicity, in this section, we consider $p = 2$ only and we will denote $S^{\mathbf{h},2}(\Omega)$ by $S^{\mathbf{h}}(\Omega)$. Let $(\lambda_{\mathbf{h}}, u_{\mathbf{h}})$ be a finite element approximation on $S_0^{\mathbf{h}}(\Omega)$, namely, $\|u_{\mathbf{h}}\|_{0,\Omega}$=1 and

$$a\big(u_{\mathbf{h}}, v\big) = \lambda_{\mathbf{h}}\big(u_{\mathbf{h}}, v\big), \quad \forall v \in S_0^{\mathbf{h}}(\Omega). \tag{4.1}$$

For clarity, we consider the approximation of any eigenvalue λ of (2.7). Here and hereafter we let $\lambda_{H\mathbf{e}}$ be the finite element eigenvalue of (4.1) corresponding to $S_0^{H\mathbf{e}}(\Omega)$ and satisfy

$$|\lambda - \lambda_{H\mathbf{e}}| \lesssim \delta_{H\mathbf{e}}^2(\lambda). \tag{4.2}$$

It is seen from Proposition 2.2 that associated with the eigenfunction $u_{H\mathbf{e}}$ satisfying (4.1) (when $\mathbf{h}$ is replaced by $H\mathbf{e}$), there exists an exact eigenfunction u of (2.7) satisfying $\|u\|_{0,\Omega} = 1$ and

$$\|u - u_{H\mathbf{e}}\|_{1,\Omega} \lesssim \delta_{H\mathbf{e}}(\lambda), \quad \|u - u_{H\mathbf{e}}\|_{0,\Omega} \lesssim H\delta_{H\mathbf{e}}(\lambda). \tag{4.3}$$

The result, which will be used in our analysis, can be derived from Riesz-Schauder theory (see, e.g., [11]).

Proposition 4.1. *Let $\mathbf{h} \in \{H, h\}^d$ and $G \subset \Omega$. If $M(\lambda) \subset H^{s+r}(G)\,(0 \le s \le 1)$, then*

$$\sup_{w\in M(\lambda),\|w\|_{0,\Omega}=1} \inf_{v\in S_0^{\mathbf{h}}(G)} \|w - v\|_{1,G} \lesssim \sigma^{r+s-1}, \tag{4.4}$$

where $\sigma = \max_{i\in\mathbb{Z}_d} \mathbf{h}^{\mathbf{e}_i}$. In particular, if $M(\lambda) \subset H^{s+2}(\Omega)\,(s \in [0,1])$, then

$$|\lambda - \lambda_{H\mathbf{e}}| \lesssim H^{2(s+1)}, \quad \|u - u_{H\mathbf{e}}\|_{1,\Omega} \lesssim H^{s+1}, \quad \|u - u_{H\mathbf{e}}\|_{0,\Omega} \lesssim H^{s+2} \tag{4.5}$$

$$\|u - P_{\mathbf{h}}u\|_{1,\Omega} \lesssim \sigma^{s+1}, \quad \|u - P_{\mathbf{h}}u\|_{0,\Omega} \lesssim \sigma^{s+2}. \tag{4.6}$$

Following the two-scale combination formula (3.1), we define the following two-scale finite element approximations to the eigenpair (λ, u) as follows (see, e.g., [21]):

$$B_{H\mathbf{e}}^h\lambda_{h\mathbf{e}} = \lambda_{H\mathbf{e}} - \sum_{i=1}^d \delta_h^{\mathbf{e}_i}\lambda_{H\mathbf{e}}, \quad B_{H\mathbf{e}}^h u_{h\mathbf{e}} = u_{H\mathbf{e}} - \sum_{i=1}^d \delta_h^{\mathbf{e}_i} u_{H\mathbf{e}}.$$

Theorem 4.1. *If $u \in H_0^1(\Omega) \cap W^{G,t+2}(\Omega)$ $(2 \le t \le 3)$, then*

$$\big|B_{H\mathbf{e}}^h\lambda_{h\mathbf{e}} - \lambda\big| \lesssim H^{t+3} + h^4, \tag{4.7}$$

$$\|B_{H\mathbf{e}}^h u_{h\mathbf{e}} - u\|_{1,\Omega} \lesssim H^{t+1} + h^2. \tag{4.8}$$

Moreover, if λ is simple, then

$$\|B_{H\mathbf{e}}^h u_{h\mathbf{e}} - u\|_{0,\Omega} \lesssim H^{t+2} + h^3. \tag{4.9}$$

Proof. From Lemma 2.1, we have

$$B_{H\mathbf{e}}^h\lambda_{h\mathbf{e}} - \lambda_{h\mathbf{e}} = \lambda\big(u, P_{h\mathbf{e}}u - B_{H\mathbf{e}}^h P_{h\mathbf{e}}u\big) + \mathcal{O}(H^6),$$

which together with Theorems 3.1 and (4.5) produces (4.7). Note that

$$\|B_{H\mathbf{e}}^h(P_{h\mathbf{e}}u - u_{h\mathbf{e}})\|_{1,\Omega} \lesssim \max_{\mathbf{h}\in\{H,h\}^d} \|P_{\mathbf{h}}u - u_{\mathbf{h}}\|_{1,\Omega}; \tag{4.10}$$

hence from the identity

$$B_{H\mathbf{e}}^h u_{h\mathbf{e}} - u = B_{H\mathbf{e}}^h\big(u_{h\mathbf{e}} - P_{h\mathbf{e}}u\big) + B_{H\mathbf{e}}^h P_{h\mathbf{e}}u - P_{h\mathbf{e}}u + P_{h\mathbf{e}}u - u, \tag{4.11}$$

we obtain (4.8) from (2.20), (3.5), and (4.5).

Now we are going to derive (4.9). From the definition of $B_{H\mathbf{e}}^h u_{h\mathbf{e}}$, we have

$$(I-\lambda K)\big(u - B_{H\mathbf{e}}^h u_{h\mathbf{e}}\big) = (I-\lambda K)\bigg(\sum_{i=1}^d (u - u_{h\mathbf{e}_i + H\hat{\mathbf{e}}_i}) - (d-1)(u - u_{H\mathbf{e}})\bigg).$$

Thus we obtain from Lemma 2.2 that

$$\begin{aligned}
&(I-\lambda K)\big(u - B_{H\mathbf{e}}^h u_{h\mathbf{e}}\big)\\
=&\sum_{i=1}^d \bigg(\frac{1}{\lambda}\big(\lambda - \lambda_{h\mathbf{e}_i + H\hat{\mathbf{e}}_i}\big)u + u - P_{h\mathbf{e}_i + H\hat{\mathbf{e}}_i}u + r_{h\mathbf{e}_i + H\hat{\mathbf{e}}_i}(u)\bigg)\\
&- (d-1)\bigg(\frac{1}{\lambda}\big(\lambda - \lambda_{H\mathbf{e}}\big)u + u - P_{H\mathbf{e}}u + r_{H\mathbf{e}}(u)\bigg)
\end{aligned}$$

or

$$\begin{aligned}
&(I-\lambda K)\big(u - B_{H\mathbf{e}}^h u_{h\mathbf{e}}\big)\\
=&\frac{1}{\lambda}\big(\lambda - B_{H\mathbf{e}}^h \lambda_{h\mathbf{e}}\big)u + u - B_{H\mathbf{e}}^h P_{h\mathbf{e}}u + \sum_{i=1}^d r_{h\mathbf{e}_i + H\hat{\mathbf{e}}_i}(u) - (d-1)r_{H\mathbf{e}}u.
\end{aligned}$$

Note that Theorems 3.1 and (4.7) lead to

$$\begin{aligned}
\bigg|\frac{1}{\lambda}\big(\lambda - B_{H\mathbf{e}}^h \lambda_{h\mathbf{e}}\big)\bigg| &\lesssim H^{t+3} + h^4,\\
\|u - B_{H\mathbf{e}}^h P_{h\mathbf{e}}u\|_{0,\Omega} &\lesssim H^{t+2} + h^3.
\end{aligned}$$

Hence using (2.33), we obtain

$$\|(I-\lambda K)\big(u - B_{H\mathbf{e}}^h u_{h\mathbf{e}}\big)\|_{0,\Omega} \lesssim H^{t+2} + h^3. \tag{4.12}$$

Denote the subspace spanned by eigenfunctions corresponding to the eigenvalue λ by H_λ. Then the assumption that λ is simple implies that $H_\lambda = \mathrm{span}\{u\}$ and

$$\big(u(B_{H\mathbf{e}}^h u_{h\mathbf{e}}, u) - B_{H\mathbf{e}}^h u_{h\mathbf{e}}, u\big) = 0,$$

namely,

$$u\big(B_{H\mathbf{e}}^h u_{h\mathbf{e}}, u\big) - B_{H\mathbf{e}}^h u_{h\mathbf{e}} \in H_\lambda^\perp \equiv \big\{v \in H_0^1(\Omega) : (u,v) = 0\big\}.$$

Note that K is a compact operator and $I - \lambda K$ is an operator from the subspace $H_\lambda^\perp$ to itself. Hence the operator $I - \lambda K$ restricted on the subspace $H_\lambda^\perp$ has a bounded inverse. Therefore, from

$$u\big(B_{H\mathbf{e}}^h u_{h\mathbf{e}}, u\big) - B_{H\mathbf{e}}^h u_{h\mathbf{e}} = (I-\lambda K)^{-1}(I-\lambda K)\big(u - B_{H\mathbf{e}}^h u_{h\mathbf{e}}\big),$$

we have

$$\|u(B^h_{H\mathbf{e}}u_{h\mathbf{e}},u)-B^h_{H\mathbf{e}}u_{h\mathbf{e}}\|_{0,\Omega}\lesssim\|(I-\lambda K)\big(u-B^h_{H\mathbf{e}}u_{h\mathbf{e}}u\big)\|_{0,\Omega},$$

which, together with (4.12), yields

$$\|u(B^h_{H\mathbf{e}}u_{h\mathbf{e}},u)-B^h_{H\mathbf{e}}u_{h\mathbf{e}}\|_{0,\Omega}\lesssim H^{t+2}+h^3. \tag{4.13}$$

Since

$$\|u-B^h_{H\mathbf{e}}u_{h\mathbf{e}}\|_{0,\Omega}\le\|u-u(B^h_{H\mathbf{e}}u_{h\mathbf{e}},u)\|_{0,\Omega}+\|u(B^h_{H\mathbf{e}}u_{h\mathbf{e}},u)-B^h_{H\mathbf{e}}u_{h\mathbf{e}}\|_{0,\Omega},$$

it remains to estimate $\|u-u(B^h_{H\mathbf{e}}u_{h\mathbf{e}},u)\|_{0,\Omega}$. Using the identity

$$1-\big(B^h_{H\mathbf{e}}u_{h\mathbf{e}},u\big)=\big(u-B^h_{H\mathbf{e}}u_{h\mathbf{e}},u\big),$$

we obtain

$$1-\big(B^h_{H\mathbf{e}}u_{h\mathbf{e}},u\big)=\frac{1}{2}\Big(\sum_{i=1}^{d}\|u_{h\mathbf{e}_i+H\hat{\mathbf{e}}_i}-u\|^2_{0,\Omega}-(d-1)\|u_{H\mathbf{e}}-u\|^2_{0,\Omega}\Big)$$

which leads to the conclusion. This completes the proof. □

From the theorems above, we can conclude that the quadratic elements may be the best choice in solving (1.1) or (2.7) taking the regularity into account.

Remark 4.1. It may be derived from Proposition 2.3 that

$$\left|\frac{a\big(B^h_{H\mathbf{e}}u_{h\mathbf{e}},B^h_{H\mathbf{e}}u_{h\mathbf{e}}\big)}{\|B^h_{H\mathbf{e}}u_{h\mathbf{e}}\|^2_{0,\Omega}}-\lambda\right|\lesssim H^{2t+2}+h^4 \tag{4.14}$$

provided $u\in H^1_0(\Omega)\cap W^{G,t+2}(\Omega)$ $\big(t\in[2,3]\big)$.

5. Numerical Examples

In this section, we shall report some numerical experiments that illustrate our two-scale discretization schemes. The numerical experiments were carried out on SGI Origin 3800 in the State Key Laboratory of Scientific and Engineering Computing, Chinese Academy of Sciences.

The first two examples are typical in quantum chemistry. For illustration, we provide numerical results for the eigenvalue approximations only.

Example 1. Consider the oscillator equation

$$-\frac{1}{2}\Delta u+\frac{1}{2}r^2u=\lambda u\quad\text{ in }\ \mathbb{R}^3, \tag{5.1}$$

where $r=\sqrt{x_1^2+x_2^2+x_3^2}$. The first four eigenvalues of (5.1) are $1.5, 2.5, 2.5$, and 2.5. In our computation, we choose $\Omega=(-5.0,5.0)^3$. The numerical results obtained by triquadratic elements and tricubic elements are provided in Table 5.1 and Table 5.2 respectively, where $l=10.0$.

It is seen from Table 5.2 that the convergence rate of tricubic elements can reach $\mathcal{O}(h^6)$; however we are not able to prove it due to the limitation of the regularity.

Although our analysis requires that the potential V is smooth, it will be shown by the next example that the two-scale discretization may work well even if the potential is not so smooth.

Table 5.1: Example 1: estimates for the first four eigenvalues by triquadratic elements.

$l/h \times l/H \times l/H$	$\lvert\lambda_1 - \lambda_{1\ H,H,H}^{h}\rvert$	$\lvert\lambda_2 - \lambda_{2\ H,H,H}^{h}\rvert$	$\lvert\lambda_3 - \lambda_{3\ H,H,H}^{h}\rvert$	$\lvert\lambda_4 - \lambda_{4\ H,H,H}^{h}\rvert$
$16 \times 4 \times 4$	0.000568817	0.135533	0.070273	0.070273
$24 \times 6 \times 6$	0.000115000	0.021530	0.010251	0.010251
$32 \times 8 \times 8$	0.000036817	0.008937	0.004633	0.004633
$48 \times 12 \times 12$	0.000007343	0.006482	0.003274	0.003274
$64 \times 16 \times 16$	0.000002320	0.002182	0.001105	0.001105
$96 \times 24 \times 24$	0.000000443	0.000451	0.000228	0.000228
convergence rate	$\mathcal{O}(h^4)$	$\mathcal{O}(h^4)$	$\mathcal{O}(h^4)$	$\mathcal{O}(h^4)$

Table 5.2: Example 1: estimates for the first four eigenvalues by tricubic elements.

$l/h \times l/H \times l/H$	$\lvert\lambda_1 - \lambda_{1\ H,H,H}^{h}\rvert$	$\lvert\lambda_2 - \lambda_{2\ H,H,H}^{h}\rvert$	$\lvert\lambda_3 - \lambda_{3\ H,H,H}^{h}\rvert$	$\lvert\lambda_4 - \lambda_{4\ H,H,H}^{h}\rvert$
$16 \times 4 \times 4$	0.000011078	0.078406	0.039263	0.039263
$24 \times 6 \times 6$	0.000001000	0.003021	0.001516	0.001516
$32 \times 8 \times 8$	0.000000209	0.001621	0.000811	0.000811
$48 \times 12 \times 12$	0.000000002	0.000173	0.000060	0.000060
convergence rate	$\mathcal{O}(h^6)$	$\mathcal{O}(h^6)$	$\mathcal{O}(h^6)$	$\mathcal{O}(h^6)$

Example 2. Consider the the Schrödinger equation of the hydrogen atom

$$-\frac{1}{2}\Delta u - \frac{1}{r}u = \lambda u \quad \text{in } \mathbb{R}^3. \tag{5.2}$$

We carry out our computation over domain $\Omega = (-6.4, 6.4)^3$. The first eigenvalue is -0.5. Due to the singularity at point $(0, 0, 0)$, we may employ a so-called graded mesh approach. The idea of graded meshes is to put the nodes of the uniform mesh graded towards the singular point, for instance, for $\Omega = (-l, l)^3$ with some singularity at $(0, 0, 0)$, we may use the nodes as

$$\widetilde{x_i} = \begin{cases} (\frac{i}{N})^{\frac{3}{2}} l, & \text{if } x_i > 0 \\ -(\frac{i}{N})^{\frac{3}{2}} l, & \text{if } x_i < 0 \end{cases} \quad \text{for } i = 1, 2, \cdots, N$$

in each coordinate direction.

The numerical results obtained by triquadratic elements and tricubic elements are presented in Table 5.3 and Table 5.4 respectively, where $\lambda_{H,H,H}^h$ represents the result of the uniform discretization, $\widetilde{\lambda}_{H,H,H}^h$ represents the result of the graded mesh and $l = 12.8$. It is seen from the numerical results that the two-scale discretization using graded mesh works successfully.

The last example is not a Schrödinger type equation.

Example 3. Consider an eigenvalue problem in three-dimensions:

$$\begin{cases} -\displaystyle\sum_{i=1}^{3} \frac{\partial}{\partial x_i}\Big(x_i^2 \frac{\partial u}{\partial x_i}\Big) = \lambda u & \text{in } \Omega = (1,3) \times (1,2) \times (1,2), \\ \qquad\qquad\qquad u = 0 & \text{on } \partial\Omega. \end{cases} \tag{5.3}$$

The first eigenvalue is

$$\lambda_1 = \frac{3}{4} + (\frac{2}{\ln^2 2} + \frac{1}{\ln^2 3})\pi^2 \simeq 50.01189403$$

and the associated eigenfunction is

$$u_1 = \prod_{i=1}^{3} \left({x_i}^{-\frac{1}{2}} \sin\Big(\frac{\pi \ln x_i}{\ln \boldsymbol{\beta}_i}\Big)\right), \qquad \beta_1 = 3,\ \beta_2 = \beta_3 = 2.$$

Table 5.3: Example 2: estimates for the first eigenvalue by triquadratic elements.

$l/h \times l/H \times l/H$	$\lvert\lambda_1 - \lambda^h_{1,H,H,H}\rvert$	$\lvert\lambda_1 - \widetilde{\lambda}^h_{1,H,H,H}\rvert$
$16 \times 4 \times 4$	0.051738	0.047198
$32 \times 8 \times 8$	0.018315	0.001536
$48 \times 12 \times 12$	0.008348	0.000405
$64 \times 16 \times 16$	0.005104	0.000200
$96 \times 24 \times 24$	0.002514	0.000143

Table 5.4: Example 2: estimates for the first eigenvalue by tricubic elements.

$l/h \times l/H \times l/H$	$\lvert\lambda_1 - \lambda^h_{1,H,H,H}\rvert$	$\lvert\lambda_1 - \widetilde{\lambda}^h_{1,H,H,H}\rvert$
$16 \times 4 \times 4$	0.036939	0.028790
$32 \times 8 \times 8$	0.018410	0.005550
$48 \times 12 \times 12$	0.009456	0.001827

Table 5.5: Example 3: results obtained by triquadratic elements.

$2/h \times 1/H \times 1/H$	$\lvert\lambda_1 - \lambda^h_{1,H,H,H}\rvert$	$\lVert u_1 - u^h_{1,H,H,H}\rVert_{1,\Omega}$	$\lVert u_1 - u^h_{1,H,H,H}\rVert_{0,\Omega}$
6×2×2	0.06386330	0.17340868	0.00452017
12×3×3	0.00487843	0.02380351	0.00034418
16×4×4	0.00142976	0.00773721	0.00006299
36×6×6	0.00024072	0.00158094	0.00000563
48×8×8	0.00016276	0.00048986	0.00000266
convergence rate	$\mathcal{O}(H^5)$	$\mathcal{O}(H^4)$	$\mathcal{O}(H^5)$

Table 5.6: Example 3: results obtained by tricubic elements.

$2/h \times 1/H \times 1/H$	$\lvert\lambda_1 - \lambda^h_{1,H,H,H}\rvert$	$\lVert u_1 - u^h_{1,H,H,H}\rVert_{1,\Omega}$	$\lVert u_1 - u^h_{1,H,H,H}\rVert_{0,\Omega}$
6×2×2	0.00238354	0.00923775	0.00114159
8×3×3	0.00032543	0.00030127	0.00005628
12×4×4	0.00027922	0.00006103	0.00000533
24×6×6	0.00022688	0.00001515	0.00000240

The numerical results obtained by triquadratic elements and tricubic elements are shown in Table 5.5 and Table 5.6, respectively. The numerical results in Table 5.5 support that our discretization scheme may be applied to other type elliptic eigenvalue equations not of Schrödinger type (cf. Appendix). It is noted that the convergence of finite element approximations in Table 5.6 is not optimal due to the regularity of the exact eigenfunction.

Remark 5.1. The ratio of h/H is chosen mainly for the optimal cost of the computation. For example, in the last example, $H = \mathcal{O}(h^{2/3})$ almost holds for the triquadratic elements, and $H = \mathcal{O}(h^{3/4})$ almost holds for the tricubic elements. But we adjust the ratio in the first two examples due to the limit of storage of the computation. Anyway, all the numerical results illustrate the efficiency of the two-scale discretization scheme.

6. Concluding Remarks

In this paper, we have proposed and analyzed the two-scale higher-order finite element discretization scheme for Schrödinger type equations. It is shown by both theory and numerics that the number of degrees of freedom of the two-scale finite element approximation is much less than that of the standard finite element solution. However, it is proved in this paper that the two-scale finite element approximation still pocesses the same approximate accuracy as that of the standard finite element solution. Hence it is a very economic solution in terms of computational cost. To apply the two-scale higher-order finite element discretization approach to solving Kohn-Sham equations in the pseudopotential setting is our on-going project. For such computations, however, there are many practical issues, including the implementation details for local density approximations, that need to be addressed. We will report our progresses in our forthcoming papers.

What we studied here is the finite element computation over tensor product domains only. Indeed, we may generalize those techniques to general domains and design some new local and parallel algorithms. We refer to [22] for relevant discussions. Finally, we should mention that the convergence of the two-scale combination approximations may be improved if the exact solution and the coefficients of the problem have better regularity.

Appendix

We may generalize the two-scale higher-order techniques to a more general eigenvalue problem on $\Omega = (0,1)^d$ as follows

$$\begin{cases} Lu = \lambda u & \text{in} \quad \Omega, \\ \;\; u = 0 & \text{on} \quad \partial\Omega, \end{cases} \tag{A.1}$$

where L is a linear elliptic operator of second order:

$$Lu = -\sum_{i,j=1}^{d} \frac{\partial}{\partial x_j}\left(a_{ij}\frac{\partial u}{\partial x_i}\right) + Vu$$

which satisfies $a_{ij} \in W^{1,\infty}(\Omega)$, $V \in W^{1,\infty}(\Omega)$, and (a_{ij}) is uniformly positive symmetric definite on $\bar{\Omega}$. The corresponding weak form is defined by:

$$a(u,v) = \int_\Omega \sum_{i,j=1}^{d} a_{ij}\frac{\partial u}{\partial x_i}\frac{\partial v}{\partial x_j} + Vuv. \tag{A.2}$$

Obviously, Proposition 2.5 is valid when $a(\cdot,\cdot)$ is defined by (A.2) and similar results to Proposition 2.6 can be also expected.

Proposition A.1. *If $w \in H_0^1(\Omega) \cap H^{p+2}(\Omega)$, then*

$$a\big((I - I_{\mathbf{h}})w, v\big) \lesssim \max_{|\boldsymbol{\alpha}|=p+1} \mathbf{h}^{\boldsymbol{\alpha}} \|w\|_{p+2,\Omega}\|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \tag{A.3}$$

Moreover, if the weak form is defined by (2.6) *and $w \in H_0^1(\Omega) \cap W^{G,p+2}(\Omega)$, then*

$$a\big((I - I_{\mathbf{h}})w, v\big) \lesssim \max_{|\boldsymbol{\alpha}|=p+1} \mathbf{h}^{\boldsymbol{\alpha}} \|w\|_{W^{G,p+2}(\Omega)}\|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \tag{A.4}$$

Proof. First of all, it is seen for any $l \in \mathbb{Z}_d$ that

$$\int_\Omega \partial_{x_l}(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_l}v = 0, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \tag{A.5}$$

If $j \in \mathbb{Z}_d \setminus \{l\}$, then we obtain from using Taylor's expansion that

$$
\begin{aligned}
&\int_\tau \partial_{x_l}(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_j}v \\
=&-\int_\tau (I - I_{\mathbf{h}\mathbf{e}_l})w\left(\sum_{i=0}^{p-1}\frac{1}{i!}(x_l - x_{\tau,l})^i\partial_{x_l}^{i+1}\partial_{x_j}v(x_{\tau,l})\right) \\
=&-\int_\tau (I - I_{\mathbf{h}\mathbf{e}_l})w\left(\sum_{i=0}^{p-2}\frac{1}{i!}(x_l - x_{\tau,l})^i\partial_{x_l}^{i+1}\partial_{x_j}v(x_{\tau,l})\right) \\
&-\int_\tau (I - I_{\mathbf{h}\mathbf{e}_l})w\frac{(x_l - x_{\tau,l})^{p-1}}{(p-1)!}\partial_{x_l}^p\partial_{x_j}v(x_{\tau,l}),
\end{aligned}
$$

which, together with integration by parts and the property of F_l, yields

$$
\begin{aligned}
&\int_\tau \partial_{x_l}(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_j}v \\
=&-\int_\tau \frac{2^p}{(2p)!}\big(F_l^p(x_l)\big)^{(p+1)}(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_l}^p\partial_{x_j}v(x_{\tau,l}) \\
&+ R_{p-1}(x_l)(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_l}^p\partial_{x_j}v(x_{\tau,l}) \\
=&(-1)^p\int_\tau \frac{2^p}{(2p)!}F_l^p(x_l)\partial_{x_l}^{p+1}(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_l}^p\partial_{x_j}v(x_{\tau,l}),
\end{aligned}
$$

or

$$
\int_\tau \partial_{x_l}(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_j}v = \frac{(-1)^p 2^p}{(2p)!}\int_\tau F_l^p(x_l)\partial_{x_l}^{p+1}w\partial_{x_l}^p\partial_{x_j}v(x_{\tau,l}).
$$

It is also observed that

$$
\begin{aligned}
\int_\Omega \partial_{x_l}(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_j}v =& \sum_{\tau\in T^{\mathbf{h}}(\Omega)}\left(\frac{(-1)^{p+1}2^p}{(2p)!}\int_\tau F_l^p(x_l)\partial_{x_l}^{p+1}\partial_{x_j}w\partial_{x_l}^p v(x_{\tau,l})\right) \\
&\lesssim h_l^{p+1}\|w\|_{W^{G,p+2}(\Omega)}\|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega),
\end{aligned} \tag{A.6}
$$

where the inverse estimate is used.

Similarly, for $w \in H_0^1(\Omega) \cap H^{p+1}(\Omega)$ and $v \in S_0^{\mathbf{h},p}(\Omega)$, we get

$$
\begin{aligned}
&\int_\tau (I - I_{\mathbf{h}\mathbf{e}_l})wv = \int_\tau \left(\sum_{i=0}^{p-2}\frac{1}{i!}(x_l - x_{\tau,l})^i(I - I_{\mathbf{h}\mathbf{e}_l})w\partial_{x_l}^i v(x_{\tau,l})\right) \\
&\quad+\int_\tau (I - I_{\mathbf{h}\mathbf{e}_l})w\frac{(x_l - x_{\tau,l})^{p-1}}{(p-1)!}\partial_{x_l}^{p-1}v(x_{\tau,l}) + \int_\tau (I - I_{\mathbf{h}\mathbf{e}_l})w\frac{(x_l - x_{\tau,l})^p}{p!}\partial_{x_l}^p v(x_{\tau,l}) \\
=&\frac{(-1)^{p-1}2^p}{(2p)!}\int_\tau F_l^p(x_l)\partial_{x_l}^{p+1}u\partial_{x_l}^{p-1}v(x_{\tau,l}) + \frac{(-1)^{p+1}2^{p+1}}{(2p+2)!}\int_\tau \big(F_l^{p+1}(x_l)\big)'\partial_{x_l}^{p+1}u\partial_{x_l}^p v(x_{\tau,l}).
\end{aligned}
$$

Thus we arrive at

$$
\begin{aligned}
\int_\Omega (I - I_{\mathbf{h}\mathbf{e}_l})wv =& \sum_{\tau\in T^{\mathbf{h}}(\Omega)}\left(\frac{(-1)^{p+1}2^p}{(2p)!}\int_\tau F_l^p(x_l)\partial_{x_l}^{p+1}w\partial_{x_l}^{p-1}v(x_{\tau,l})\right. \\
&\left.+\frac{(-1)^{p+1}2^{p+1}}{(2p+2)!}\int_\tau \big(F_l^{p+1}(x_l)\big)'\partial_{x_l}^{p+1}w\partial_{x_l}^p v(x_{\tau,l})\right).
\end{aligned} \tag{A.7}
$$

Obviously, substituting w by $\partial_{x_i} w$ and v by $\partial_{x_j} v$ in (A.7) implies

$$\int_\Omega \partial_{x_i}(I - I_{\mathbf{he}_l}) w \partial_{x_j} v \lesssim h_l^{p+1} \|w\|_{W^{G,p+2}(\Omega)} \|v\|_{1,\Omega}, \quad i \neq l. \tag{A.8}$$

Therefore, it follows from (A.5), (A.6) and (A.8) that

$$\begin{aligned} &\int_\Omega a_{ij} \partial_{x_i}(I - I_{\mathbf{he}_l}) w \partial_{x_j} v \\ &= a_{ij}(x_\tau) \int_\Omega \partial_{x_i}\big(I - I_{\mathbf{he}_l}) w \partial_{x_j} v + \int_\Omega (a_{ij} - a_{ij}(x_\tau)) \partial_{x_i}(I - I_{\mathbf{he}_l}) w \partial_{x_j} v \\ &\lesssim h_l^{p+1} \|w\|_{p+2,\Omega} \|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \end{aligned} \tag{A.9}$$

Combining (A.9) and

$$\int_\Omega V(I - I_{\mathbf{he}_l}) wv \lesssim h_l^{p+1} \|w\|_{p+1,\Omega} \|v\|_{0,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega), \tag{A.10}$$

we have

$$a\big((I - I_{\mathbf{he}_l}) w, v\big) \lesssim h_l^{p+1} \|w\|_{p+2,\Omega} \|v\|_{1,\Omega}, \quad \forall v \in S_0^{\mathbf{h},p}(\Omega). \tag{A.11}$$

Note that from the identity

$$I - I_{\mathbf{h}} = - \sum_{0 \le \boldsymbol{\alpha} \le \mathbf{e}, |\boldsymbol{\alpha}| \ge 1} (-1)^{|\boldsymbol{\alpha}|} \prod_{0 \le \boldsymbol{\beta} \le \boldsymbol{\alpha}, |\boldsymbol{\beta}| = 1} (I - I_{\mathbf{h}\boldsymbol{\beta}}),$$

we obtain for any $v \in S_0^{\mathbf{h},p}(\Omega)$ that

$$\begin{aligned} a\big((I - I_{\mathbf{h}}) w, v\big) = &\sum_{0 \le \boldsymbol{\alpha} \le \mathbf{e}, |\boldsymbol{\alpha}| = 1} a\big((I - I_{\mathbf{h}\boldsymbol{\alpha}}) w, v\big) \\ &- \sum_{0 \le \boldsymbol{\alpha} \le \mathbf{e}, |\boldsymbol{\alpha}| \ge 2} (-1)^{|\boldsymbol{\alpha}|} a\bigg(\prod_{0 \le \boldsymbol{\beta} \le \boldsymbol{\alpha}, |\boldsymbol{\beta}| = 1} (I - I_{\mathbf{h}\boldsymbol{\beta}}) w, v\bigg). \end{aligned} \tag{A.12}$$

Hence we can derive (A.3) from (2.36), (A.11) and (A.12). Moreover, (A.4) can be obtained using (2.36), (A.5), (A.6) and (A.8). This completes the proof. □

Consequently, we have the following results.

Theorem A.1. *If $u \in H_0^1(\Omega) \cap H^{p+2}(\Omega)$, then*

$$\|B_{H\mathbf{e}}^h P_{h\mathbf{e}} u - P_{h\mathbf{e}} u\|_{0,\Omega} + H \|B_{H\mathbf{e}}^h P_{h\mathbf{e}} u - P_{h\mathbf{e}} u\|_{1,\Omega} \lesssim H^{p+2}. \tag{A.13}$$

Moreover,

$$\|B_{H\mathbf{e}}^h P_{h\mathbf{e}} u - P_{h\mathbf{e}} u\|_{1-p,\Omega} \lesssim H^{2p+1}, \quad p = 2, 3. \tag{A.14}$$

Theorem A.2. *If $u \in H_0^1(\Omega) \cap H^4(\Omega)$ and $p = 2$, then*

$$\big|B_{H\mathbf{e}}^h \lambda_{h\mathbf{e}} - \lambda_{h\mathbf{e}}\big| \lesssim H^5, \quad \|B_{H\mathbf{e}}^h u_{h\mathbf{e}} - u_{h\mathbf{e}}\|_{1,\Omega} \lesssim H^3. \tag{A.15}$$

Moreover, if λ is simple, then

$$\|u - B_{H\mathbf{e}}^h u_{h\mathbf{e}}\|_{0,\Omega} \lesssim H^4 + h^3. \tag{A.16}$$

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