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Moritz Hauck, Yizhou Liang

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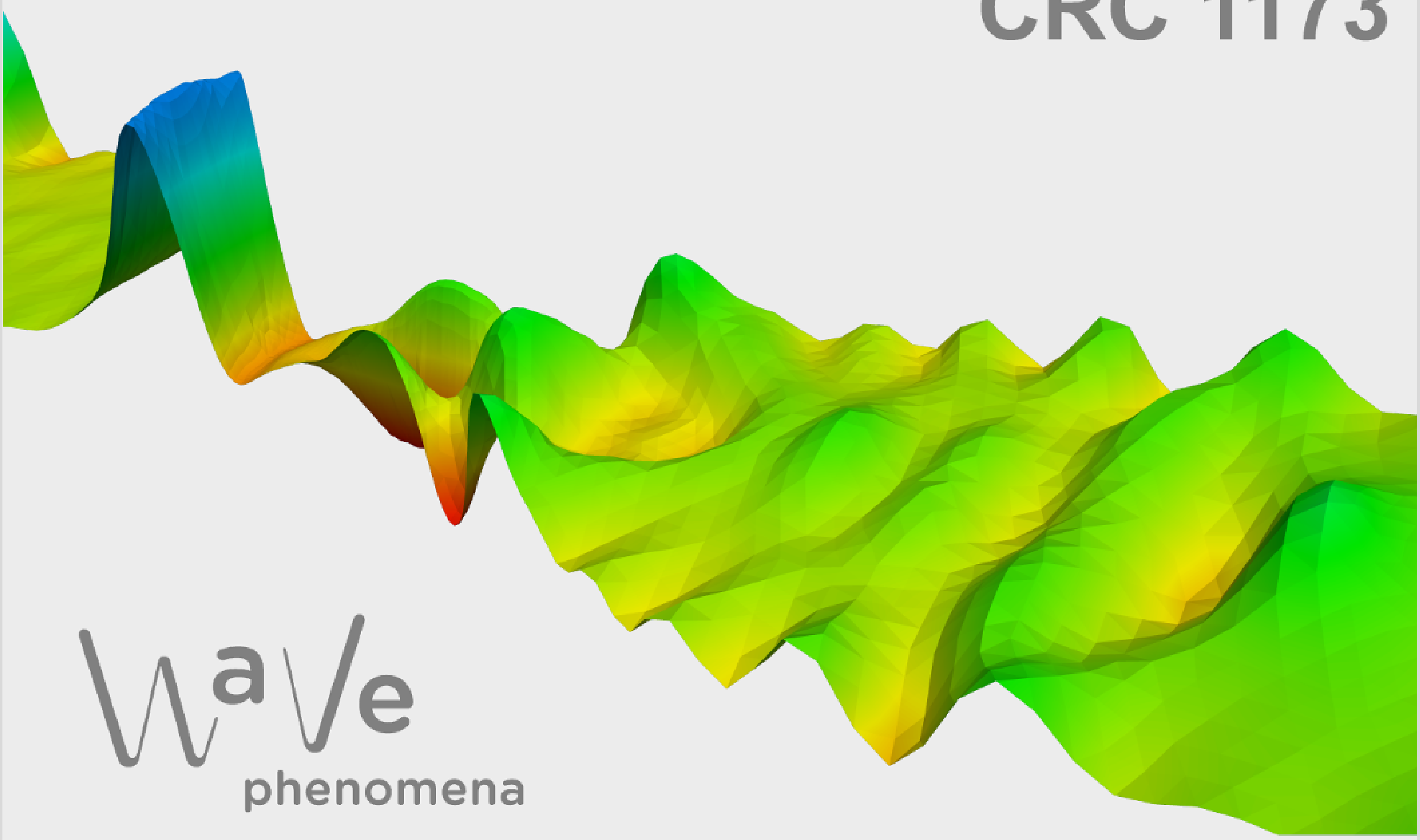

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A HYBRID HIGH-ORDER METHOD FOR THE GROSS–PITAEVSKII EIGENVALUE PROBLEM

MORITZ HAUCK*, YIZHOU LIANG†

ABSTRACT. We introduce a hybrid high-order method for approximating the ground state of the nonlinear Gross–Pitaevskii eigenvalue problem. Optimal convergence rates are proved for the ground state approximation, as well as for the associated eigenvalue and energy approximations. Unlike classical conforming methods, which inherently provide upper bounds on the ground state energy, the proposed approach gives rise to guaranteed and asymptotically exact lower energy bounds. Importantly, and in contrast to previous works, they are obtained directly without the need of post-processing, leading to more accurate guaranteed lower energy bounds in practice.

1. INTRODUCTION

The Gross–Pitaevskii eigenvalue problem (GP-EVP) arises in quantum physics, where it describes stationary quantum states of bosonic particles at ultracold temperatures, known as Bose–Einstein condensates; see, e.g., [DGPS99, ASRVK01, Fet09]. The problem involves a non-negative trapping potential $V \in L^\infty(\Omega)$ and a parameter $\kappa > 0$ describing the strength of the repulsive particle interactions. As computational domain we consider a bounded convex Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, where we note that the restriction to a sufficiently large domain, along with homogeneous Dirichlet boundary conditions, is a standard and physically reasonable assumption for modeling low-energy quantum states, cf. [BC13]. Mathematically, the GP-EVP seeks L^2-normalised eigenfunctions $\{u_j : j = 1, 2, \dots\} \subset H_0^1(\Omega)$ and corresponding eigenvalues $\{\lambda_j : j = 1, 2, \dots\}$ such that

$$-\Delta u_j + V u_j + \kappa |u_j|^2 u_j = \lambda_j u_j \tag{1.1}$$

holds in the weak sense. The function $|u_j|^2$ represents the density of the stationary quantum state u_j, and the eigenvalue λ_j is typically called the chemical potential. It is a classical result that all eigenvalues of (1.1) are real and positive, and the smallest eigenvalue is simple; see, e.g., [CCM10]. Without loss of generality, we assume that the eigenvalues are ordered nondecreasingly, i.e., $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots$.

The GP-EVP arises as the Euler–Lagrange equations for critical points of the Gross–Pitaevskii energy, defined for all $v \in H_0^1(\Omega)$ as,

$$\mathcal{E}(v) \coloneqq \tfrac{1}{2}(\nabla v, \nabla v)_{L^2} + \tfrac{1}{2}(Vv, v)_{L^2} + \tfrac{\kappa}{4}(|v|^2 v, v)_{L^2}, \tag{1.2}$$

subject to the L^2-normalisation constraint. The ground state, which represents the stationary quantum state of lowest energy, is characterised as the minimiser of the Gross–Pitaevskii energy, i.e.,

$$u \in \operatorname*{arg\,min}_{v \in H_0^1(\Omega)\,:\, \|v\|_{L^2} = 1} \mathcal{E}(v). \tag{1.3}$$

We emphasise that, under the above assumptions on Ω and V, the constrained minimisation problem (1.3) admits a unique global minimiser (up to sign). Moreover,

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this ground state u coincides, up to sign, with the eigenfunction u_1 associated with the smallest eigenvalue λ_1 of (1.1). The minimal energy $E := \mathcal{E}(u)$ is related to the smallest eigenvalue by the identity $\lambda_1 = 2E + \frac{\kappa}{2}\|u\|_{L^4}^4$. For further theoretical results on the Gross–Pitaevskii problem, see, for example, [CCM10].

A wide range of discretisation methods has been proposed in the literature to approximate the Gross–Pitaevskii ground state. Most existing approaches are based on H^1_0-conforming discretisations, including standard continuous finite elements [Zho04, CCM10, CHZ11], spectral and pseudospectral methods [CCM10, BC13], multiscale methods [HMP14, HW22, HP23, PWZ24], and mesh-adaptive methods [DH10, HSW21]. Recently, also non-standard conforming finite element methods using mass lumping techniques to preserve certain positivity properties of the ground state have been introduced; see [CLLZ24, HLP24]. A characteristic property of conforming discretisations is that they approximate the ground state energy from above, as the energy functional is minimised over a subset. In the context of linear eigenvalue problems, where the terms energy and eigenvalue can be used interchangeably, several strategies have been developed to compute lower eigenvalue bounds. Among these, mixed finite element methods have proven effective [Gal23], and this approach has recently been extended to the present nonlinear GP-EVP in [GHLP25]. However, this method typically requires an additional postprocessing step to obtain asymptotically exact lower bounds. An alternative approach that gives guaranteed lower eigenvalue bounds without the need for postprocessing is provided by hybrid high-order (HHO) methods; see [DPT18] for an overview. In the linear setting, such bounds have been established, for example in [CEP21, CGT24, Tra24]; see also [CZZ20] for a similar result based on the related hybridisable discontinuous Galerkin method.

In this work, we extend the HHO methodology to the GP-EVP, aiming to obtain guaranteed lower bounds on the ground state energy without the need for post-processing. To this end, we introduce a modified version of the HHO method that employs a lowest-order quadrature rule for the nonlinearity. This modification is crucial for estimating the nonlinear term in the proof of the guaranteed lower energy bound via Jensen's inequality. Note that the lack of higher-order generalisations of Jensen's inequality prevents us from deriving high-order guaranteed lower energy bounds for the Gross–Pitaevskii problem. Although the guaranteed lower energy bounds we obtain are only of lowest order, they can still be significantly more accurate than those from the post-processed lowest-order mixed discretization in [GHLP25]. The improved accuracy is due to the absence of post-processing, which can degrade the quality of the bounds, particularly for smooth problems where discretization errors are comparatively small. Numerical experiments clearly demonstrate this improvement, showing that the guaranteed lower energy bounds of the proposed modified HHO method are more accurate by up to two orders of magnitude than the post-processed mixed discretisation from [GHLP25].

In addition to providing guaranteed lower energy bounds, HHO methods offer improved convergence rates for the reconstructed unknowns compared to classical finite element methods. Specifically, when using k-th order polynomials on the mesh faces and assuming sufficient smoothness, the reconstructed ground state approximation exhibits optimal convergence rates of order $k+1$ in the H^1-seminorm and $k+2$ in the L^2-norm. We provide a rigorous convergence analysis establishing these rates, along with optimal convergence of order $2k+2$ for the energy and eigenvalue approximations. Furthermore, we analyse the convergence of the proposed modified HHO method and prove first-order H^1-convergence of the ground state approximation, second-order L^2-convergence, and second-order convergence for the energy and eigenvalue approximations. Notably, the presented error analysis differs substantially from standard techniques in the linear setting. Instead, it is inspired by the analysis conducted in [CCM10, GHLP25] for classical conforming and mixed discretisations of the Gross–Pitaevskii problem, respectively.

The remainder of the paper is organised as follows. Section 2 introduces the HHO method for the Gross–Pitaevskii problem. Guaranteed lower energy bounds for a modified HHO method are established in Section 3. Section 4 presents an a priori convergence analysis of the HHO method and its modified version. Numerical experiments supporting our theoretical results are presented in Section 5.

2. Hybrid high-order method

Consider a hierarchy of simplicial meshes $\{\mathcal{T}_h\}_{h>0}$ of the domain Ω, which we assume to be geometrically conforming and shape regular. We denote by T the elements of $\mathcal{T}_h$, and define the maximal mesh size of $\mathcal{T}_h$ as $h \coloneqq \max_{T\in\mathcal{T}_h} h_T$, where $h_T \coloneqq \mathrm{diam}(T)$. The set of mesh faces of $\mathcal{T}_h$, denoted by $\mathcal{F}_h$, is partitioned into the set of interior faces $\mathcal{F}_h^i$ and boundary faces $\mathcal{F}_h^b$. For any $T \in \mathcal{T}_h$, we denote by $\mathcal{F}_{\partial T}$ the set of faces lying on the boundary of T. The space of polynomials of total degree at most $l \in \mathbb{N}_0$ on an element $T \in \mathcal{T}_h$ is denoted by $\mathcal{P}^l(T)$. Similarly, $\mathcal{P}^k(F)$ denotes the space of polynomials of total degree at most $k \in \mathbb{N}_0$ on a face $F \in \mathcal{F}_h$. Moreover, for any $T \in \mathcal{T}_h$, the space of broken polynomials on ∂T is defined as

$$\mathcal{P}^k(\mathcal{F}_{\partial T}) \coloneqq \left\{v \in L^2(\partial T) \,:\, v|_F \in \mathcal{P}^k(F),\ \forall F \in \mathcal{F}_{\partial T}\right\}.$$

We further introduce for all $T \in \mathcal{T}_h$ and all $F \in \mathcal{F}_h$ the projections $\Pi_T^l\colon L^2(T) \to \mathcal{P}^l(T)$ and $\Pi_F^k\colon L^2(F) \to \mathcal{P}^k(F)$, which are defined as orthogonal projections with respect to the L^2-inner products $(\cdot,\cdot)_T$ and $(\cdot,\cdot)_F$, respectively.

Global discrete polynomial spaces can be obtained by concatenating the local spaces $\mathcal{P}^l(T)$ and $\mathcal{P}^k(F)$ in a discontinuous manner, which gives

$$\mathcal{P}^l(\mathcal{T}_h) \coloneqq \{v \in L^2(\Omega) \,:\, v|_T \in \mathcal{P}^l(T),\ \forall T \in \mathcal{T}_h\},$$
$$\mathcal{P}^k(\mathcal{F}_h) \coloneqq \{v \in L^2(\Sigma) \,:\, v|_F \in \mathcal{P}^k(F),\ \forall F \in \mathcal{F}_h\},$$

where $\Sigma \coloneqq \cup_{F\in\mathcal{F}_h} F$ denotes the mesh skeleton. Corresponding L^2-projections can be defined piecewise as follows: $\Pi^l_{\mathcal{T}_h}: L^2(\Omega) \to \mathcal{P}^l(\mathcal{T}_h)$ by $(\Pi^l_{\mathcal{T}_h}\cdot)|_T \coloneqq \Pi^l_T\cdot$ for all $T \in \mathcal{T}_h$, and $\Pi^k_{\mathcal{F}_h}: L^2(\Sigma) \to \mathcal{P}^k(\mathcal{F}_h)$ by $(\Pi^k_{\mathcal{F}_h}\cdot)|_F \coloneqq \Pi^k_F\cdot$ for all $F \in \mathcal{F}_h$.

The global approximation space of the HHO method is given by

$$\hat{V}_h \coloneqq \mathcal{P}^{k+1}(\mathcal{T}_h) \times \mathcal{P}^k(\mathcal{F}_h), \tag{2.1}$$

where we choose $l = k+1$, which is a classical choice for HHO methods in the context of guaranteed lower eigenvalue bounds. Note that the hat notation emphasises the presence of both element and face components. For a function $\hat{v}_h \in \hat{V}_h$, these components are denoted by $\hat{v}_h = (v_{\mathcal{T}_h}, v_{\mathcal{F}_h})$, with $v_{\mathcal{T}_h} = (v_T)_{T\in\mathcal{T}_h}$ and $v_{\mathcal{F}_h} = (v_F)_{F\in\mathcal{F}_h}$. Furthermore, for any element $T \in \mathcal{T}_h$, we denote the corresponding restriction of a function $\hat{v}_h \in \hat{V}_h$ by $\hat{v}_T = (v_T, v_{\partial T}) \in \hat{V}_T \coloneqq \mathcal{P}^{k+1}(T) \times \mathcal{P}^k(\mathcal{F}_{\partial T})$, where $v_{\partial T}$ is given, for any $F \in \mathcal{F}_{\partial T}$, as $v_{\partial T}|_F = v_F$. The subspace of $\hat{V}_h$ incorporating homogeneous Dirichlet boundary conditions is defined as

$$\hat{U}_h \coloneqq \{\hat{v}_h \in \hat{V}_h \,:\, v_F = 0,\ \forall F \in \mathcal{F}_h^b\}. \tag{2.2}$$

A central component of the HHO methodology is the reconstruction operator $\mathcal{R}_h\colon \hat{V}_h \to \mathcal{P}^{k+1}(\mathcal{T}_h)$. Given $\hat{v}_h \in \hat{V}_h$, its reconstruction $\mathcal{R}_h\hat{v}_h \in \mathcal{P}^{k+1}(\mathcal{T}_h)$ is defined as the unique function satisfying, for all $T \in \mathcal{T}_h$ and $\varphi \in \mathcal{P}^{k+1}(T)$,

$$(\nabla(\mathcal{R}_h\hat{v}_h)|_T, \nabla\varphi)_{L^2(T)} = -(v_T, \Delta\varphi)_{L^2(T)} + (v_{\partial T}, \partial_n\varphi)_{L^2(\partial T)}, \tag{2.3a}$$

$$((\mathcal{R}_h\hat{v}_h)|_T, 1)_{L^2(T)} = (v_T, 1)_{L^2(T)}, \tag{2.3b}$$

where ∂_n denotes the outward normal derivative on ∂T.

Having introduced the reconstruction operator, we now introduce the discrete bilinear form of the HHO method. For a given stabilisation parameter $\sigma > 0$, it is defined for all $\hat{v}_h, \hat{\varphi}_h \in \hat{V}_h$ by

$$a_h(\hat{v}_h, \hat{\varphi}_h) \coloneqq (\nabla_h \mathcal{R}_h \hat{v}_h, \nabla_h \mathcal{R}_h \hat{\varphi}_h)_{L^2} + s_h(\hat{v}_h, \hat{\varphi}_h),$$

where ∇_h denotes the $\mathcal{T}_h$-piecewise gradient. The stabilisation bilinear form s_h is given by $s_h(\hat{v}_h, \hat{\varphi}_h) \coloneqq \sum_{T\in\mathcal{T}_h} s_T(\hat{v}_T, \hat{\varphi}_T)$ with s_T for all $\hat{v}_T, \hat{\varphi}_T \in \hat{V}_T$ defined as

$$s_T(\hat{v}_T, \hat{\varphi}_T) \coloneqq \sigma \sum_{F\in\mathcal{F}_{\partial T}} \Big\{ \ell_{T,F}^{-1} \left(\Pi_F^k \left(v_{\partial T} - (\mathcal{R}_h \hat{v}_h)_T\right), \Pi_F^k \left(\varphi_{\partial T} - (\mathcal{R}_h \hat{\varphi}_h)_T\right)\right)_{L^2(F)} \Big\} + \sigma h_T^{-2} \left(v_T - (\mathcal{R}_h \hat{v}_h)_T, \varphi_T - (\mathcal{R}_h \hat{\varphi}_h)_T\right)_{L^2(T)}.$$

Here, the weights $\ell_{T,F} > 0$ are for any $T \in \mathcal{T}_h$ and $F \in \mathcal{F}_{\partial T}$ defined as

$$\ell_{T,F} \coloneqq \frac{|F|_{d-1}\, h_T^2}{|T_F|_d},$$

where $T_F \coloneqq \operatorname{conv}\{x_T, F\} \subset T$ is the convex hull of x_T, denoting the barycenter of the element T, and the face F. Further, $|S|_n$ for $n \in \{1, \dots, d\}$ denotes the n-dimensional volume of the set S. Due to shape regularity of $\mathcal{T}_h$, we have the scaling $\ell_{T,F} \approx h_T$. The bilinear form s_h serves to penalise the non-conformity of the discrete solution $\hat{u}_h = (u_{\mathcal{T}_h}, u_{\mathcal{F}_h})$, in particular the discrepancy between $u_{\mathcal{T}_h}$ and $u_{\mathcal{F}_h}$ across the mesh skeleton Σ. Note that the above choice of stabilisation was introduced in the context of guaranteed lower eigenvalue bounds in [Tra24, Eq. (3.6)], and a related stabilisation for the case $l = k$ was proposed in [DPD20, Ex. 2.8]. The latter stabilisation, however, is unstable for our choice $l = k + 1$, cf. [Tra24]. The discrete bilinear forms a_h and s_h induce corresponding discrete (semi-)norms, defined by $\|\cdot\|_{a_h}^2 \coloneqq a_h(\cdot,\cdot)$ and $|\cdot|_{s_h}^2 \coloneqq s_h(\cdot,\cdot)$, respectively.

A discrete counterpart of the energy (1.2) can be defined, for any $\hat{v}_h \in \hat{U}_h$, as

$$\mathcal{E}_h(\hat{v}_h) \coloneqq \tfrac{1}{2} a_h(\hat{v}_h, \hat{v}_h) + \tfrac{1}{2}(V v_{\mathcal{T}_h}, v_{\mathcal{T}_h})_{L^2} + \tfrac{\kappa}{4}(|v_{\mathcal{T}_h}|^2 v_{\mathcal{T}_h}, v_{\mathcal{T}_h})_{L^2},$$

and the resulting HHO approximation $\hat{u}_h \in \hat{U}_h$ to the ground state u is characterised as the solution to the following discrete constrained minimisation problem:

$$\hat{u}_h \in \operatorname*{arg\,min}_{\hat{v}_h \in \hat{U}_h \,:\, \|v_{\mathcal{T}_h}\|_{L^2} = 1} \mathcal{E}_h(\hat{v}_h), \tag{2.4}$$

where $E_h \coloneqq \mathcal{E}_h(\hat{u}_h)$ denotes the corresponding discrete ground state energy. Unlike the continuous case, where the ground state is unique up to sign, uniqueness properties in the discrete setting remain an open question, with results only known for the first-order lumped continuous finite element method, cf. [CLLZ24, HLP24]. Nevertheless, this non-uniqueness is typically not problematic in practice, and we proceed under the assumption that a discrete minimiser has been found. Such a discrete minimiser always exists by finite-dimensional compactness arguments (Bolzano-Weierstrass theorem). To align the sign of the discrete solution with that of the continuous ground state u, we choose the sign of $\hat{u}_h$ such that $(u, u_{\mathcal{T}_h})_{L^2} \geq 0$.

3. Guaranteed lower energy bound

Due to the nonlinearity, classical techniques for obtaining guaranteed lower eigenvalue bounds with HHO methods are not directly applicable. The approach in [GHLP25], which establishes such bounds for the Gross–Pitaevskii problem using lowest-order mixed finite elements and a post-processing step, relies on Jensen's inequality to handle the nonlinearity. This is feasible because the ground state is approximated by $\mathcal{T}_h$-piecewise constants and Jensen's inequality is applicable in this setting. However, for the HHO method defined in (2.4), it is unclear how to apply Jensen's inequality, since the bulk approximation space consists at least of $\mathcal{T}_h$-piecewise first-order polynomials. Corresponding generalizations of Jensen's inequality are not known (and also not expected to hold).

To still obtain a guaranteed lower energy bound using the HHO methodology, we introduce a modified discrete energy functional, defined for all $\hat{v}_h \in \hat{U}_h$ as

$$\mathcal{E}_h^0(\hat{v}_h) \coloneqq \tfrac{1}{2} a_h(\hat{v}_h, \hat{v}_h) + \tfrac{1}{2}(V v_{\mathcal{T}_h}, v_{\mathcal{T}_h})_{L^2} + \tfrac{\kappa}{4}(|\Pi^0_{\mathcal{T}_h} v_{\mathcal{T}_h}|^2 v_{\mathcal{T}_h}, v_{\mathcal{T}_h})_{L^2}. \tag{3.1}$$

The special treatment of the nonlinearity can be interpreted as applying a low-order quadrature rule to (parts of) the nonlinear term. The corresponding modified HHO approximation $\hat{u}_h^0 \in \hat{U}_h$ is then defined as the solution to:

$$\hat{u}_h^0 \in \operatorname*{arg\,min}_{\hat{v}_h \in \hat{U}_h \,:\, \|v_{\mathcal{T}_h}\|_{L^2}=1} \mathcal{E}_h^0(\hat{v}_h). \tag{3.2}$$

Note that the modified HHO approximation is considered only for $k = 0$, as the low-order quadrature in (3.2) prevents any gain in convergence rates for $k > 0$.

To derive guaranteed lower energy bounds, one typically exploits the minimising property of (3.2) by bounding the discrete energy from above through evaluating the discrete energy functional at a suitable interpolation of the exact solution. For this purpose, we introduce an interpolation operator as

$$\mathcal{I}_h \colon H^1_0(\Omega) \to \hat{U}_h, \qquad \mathcal{I}_h v \coloneqq \big(\Pi^{k+1}_{\mathcal{T}_h} v,\, \Pi^k_{\mathcal{F}_h} v\big).$$

The following important operator identity holds:

$$\mathcal{R}_h \circ \mathcal{I}_h = \mathcal{G}_h, \tag{3.3}$$

where $\mathcal{G}_h \colon H^1_0(\Omega) \to \mathcal{P}^{k+1}(\mathcal{T}_h)$ denotes the elliptic projection. Given a function $v \in H^1_0(\Omega)$, its elliptic projection $\mathcal{G}_h v \in \mathcal{P}^{k+1}(\mathcal{T}_h)$ is defined as the unique function satisfying, for all $T \in \mathcal{T}_h$ and $w \in \mathcal{P}^{k+1}(T)$, the two conditions

$$(\nabla(\mathcal{G}_h v)|_T, \nabla w)_{L^2(T)} = (\nabla v, \nabla w)_{L^2(T)}, \tag{3.4a}$$

$$((\mathcal{G}_h v)|_T, 1)_{L^2(T)} = (v, 1)_{L^2(T)}. \tag{3.4b}$$

The desired guaranteed lower energy bound for the modified HHO approximation is stated in the following theorem.

Theorem 3.1 (Guaranteed lower energy bound)**.** *Assume that $V \in \mathcal{P}^0(\mathcal{T}_h)$ and let the stabilisation parameter σ and the mesh size h be chosen such that*

$$1 - \sigma(\tfrac{1}{\pi^2} + C_{\mathrm{tr}}) - \tfrac{4h^2 E_h^0}{\pi^2} \geq 0 \tag{3.5}$$

with the constant $C_{\mathrm{tr}} \coloneqq 1/\pi^2 + 2/(d\pi) > 0$. Then, there holds the following guaranteed lower energy bound:

$$E_h^0 \leq E.$$

Proof. The discrete energy of the ground state approximation $\hat{u}_h^0$ from (3.2) is characterised by the pseudo-Rayleigh quotient

$$E_h^0 = \min_{\hat{v}_h \in \hat{U}_h \,:\, \|v_{\mathcal{T}_h}\|_{L^2}>0} \frac{1}{\|v_{\mathcal{T}_h}\|^4_{L^2}} \Big\{ \tfrac{1}{2}(\nabla_h \mathcal{R}_h \hat{v}_h, \nabla_h \mathcal{R}_h \hat{v}_h)_{L^2} \|v_{\mathcal{T}_h}\|^2_{L^2}$$
$$+ \tfrac{1}{2} s_h(\hat{v}_h, \hat{v}_h)\|v_{\mathcal{T}_h}\|^2_{L^2} + \tfrac{1}{2}(V v_{\mathcal{T}_h}, v_{\mathcal{T}_h})_{L^2}\|v_{\mathcal{T}_h}\|^2_{L^2} + \tfrac{\kappa}{4}(|\Pi^0_{\mathcal{T}_h} v_{\mathcal{T}_h}|^2 v_{\mathcal{T}_h}, v_{\mathcal{T}_h})_{L^2} \Big\}.$$

Next, we majorize E_h^0 by choosing $\hat{v}_h = \mathcal{I}_h u \in \hat{U}_h$ and use (3.3), which results in

$$E_h^0 \|\Pi^{k+1}_{\mathcal{T}_h} u\|^4_{L^2} \leq \tfrac{1}{2}(\nabla_h \mathcal{G}_h u, \nabla_h \mathcal{G}_h u)_{L^2}\|\Pi^{k+1}_{\mathcal{T}_h} u\|^2_{L^2} + \tfrac{1}{2} s_h(\mathcal{I}_h u, \mathcal{I}_h u)\|\Pi^{k+1}_{\mathcal{T}_h} u\|^2_{L^2}$$
$$+ \tfrac{1}{2}(V \Pi^{k+1}_{\mathcal{T}_h} u, \Pi^{k+1}_{\mathcal{T}_h} u)_{L^2}\|\Pi^{k+1}_{\mathcal{T}_h} u\|^2_{L^2} + (|\Pi^0_{\mathcal{T}_h} u|^2 \Pi^{k+1}_{\mathcal{T}_h} u, \Pi^{k+1}_{\mathcal{T}_h} u)_{L^2}..$$

In the following, we bound all the terms on the right-hand side of the latter inequality individually, where we note that $\|\Pi_{\mathcal{T}_h}^{k+1}u\|_{L^2}^2 \leq \|u\|_{L^2}^2 = 1$. For the first term, we obtain using Pythagoras theorem, that

$$(\nabla_h \mathcal{G}_h u, \nabla_h \mathcal{G}_h u)_{L^2} = \|\nabla u\|_{L^2}^2 - \|\nabla_h (u - \mathcal{G}_h u)\|_{L^2}^2.$$

The second term can be estimated using (3.3), Lemmas A.1 and A.2, and the stability properties of the L^2-projections $\Pi_{\mathcal{T}_h}^{k+1}$ and $\Pi_{\mathcal{F}_h}^{k}$, as

$$s_h(\mathcal{I}_h u, \mathcal{I}_h u) \leq \sigma(\tfrac{1}{\pi^2} + C_{\mathrm{tr}})\|\nabla_h (u - \mathcal{G}_h u)\|_{L^2}^2.$$

For estimating the third term, let us recall that $V \in \mathcal{P}^0(\mathcal{T}_h)$. This allows to split up the L^2-inner product into local element contributions. Using the local stability properties of Π_T^{k+1}, this yields that

$$(V \Pi_{\mathcal{T}_h}^{k+1} u, \Pi_{\mathcal{T}_h}^{k+1} u)_{L^2} = \sum_{T \in \mathcal{T}_h} V|_T \|\Pi_T^{k+1} u\|_{L^2(T)}^2 \leq (Vu, u)_{L^2}.$$

To estimate the fourth term, we again split up the inner product in local element contributions. Noting that $\Pi_T^0 \Pi_T^{k+1} v = \Pi_T^0 v$ for all $v \in L^2(T)$, we obtain with Jensen's inequality for all $T \in \mathcal{T}_h$ that

$$(|\Pi_T^0 u|^2 \Pi_T^{k+1} u, \Pi_T^{k+1} u)_T \leq \Big(\fint_T u \,\mathrm{d}x\Big)^2 (u,u)_T \leq |T|_d \Big(\fint_T u^2 \,\mathrm{d}x\Big)^2 \leq (|u|^2 u, u)_T.$$

Summing up over all $T \in \mathcal{T}_h$ then results in

$$(|\Pi_{\mathcal{T}_h}^0 u|^2 \Pi_{\mathcal{T}_h}^{k+1} u, \Pi_{\mathcal{T}_h}^{k+1} u)_{L^2} \leq (|u|^2 u, u)_{L^2}.$$

Combining the previous estimates gives

$$E_h^0 \|\Pi_{\mathcal{T}_h}^{k+1} u\|_{L^2}^4 \leq E - \tfrac{1}{2}\big(1 - \sigma(\tfrac{1}{\pi^2} + C_{\mathrm{tr}})\big)\|\nabla_h (u - \mathcal{G}_h u)\|_{L^2}^2. \tag{3.6}$$

For rewriting the left-hand side of (3.6), we use the Pythagorean identity and the best-approximation property of the L^2-projection $\Pi_{\mathcal{T}_h}^{k+1}$ and Lemma A.1 to get that

$$\begin{aligned}\|\Pi_{\mathcal{T}_h}^{k+1} u\|_{L^2}^4 &= \big(\|u\|_{L^2}^2 - \|u - \Pi_{\mathcal{T}_h}^{k+1} u\|_{L^2}^2\big)^2 \geq \big(1 - \|u - \mathcal{G}_h u\|_{L^2}^2\big)^2 \\ &\geq 1 - \tfrac{2h^2}{\pi^2}\|\nabla_h (u - \mathcal{G}_h u)\|_{L^2}^2.\end{aligned}$$

Finally, the combination of the previous estimates leads to the inequality

$$E_h^0 \leq E - \tfrac{1}{2}\big(1 - \sigma(\tfrac{1}{\pi^2} + C_{\mathrm{tr}}) - \tfrac{4h^2 E_h^0}{\pi^2}\big)\|\nabla_h (u - \mathcal{G}_h u)\|_{L^2}^2,$$

which completes the proof. □

Remark 3.2 (Assumption of $\mathcal{T}_h$-piecewise constant potentials). The assumption $V \in \mathcal{P}^0(\mathcal{T}_h)$ in Theorem 3.1 is essential for proving the guaranteed lower energy bound. For simple potentials, where the minimum value on each element can be easily computed (e.g., the harmonic potential $V(x) = \frac{1}{2}|x|^2$), one can approximate V by a piecewise constant function that assigns this minimum value to each element. Applying the modified HHO method (3.2) to this piecewise constant potential approximation then yields a guaranteed lower energy bound for the original problem.

4. A priori error analysis

In this section, we present an a priori error analysis of the HHO approximation introduced in (2.4) and its modified version from (3.2). The analysis is inspired by the works [Zho04, CCM10] on classical conforming finite element methods. Results from the conforming setting are used at several points in the analysis, along with technical tools that enable their application in the present non-conforming setting.

The Euler–Lagrange equations associated with the constrained minimisation problem (1.3) give rise to the following eigenvalue problem: seek $(u, \lambda) \in H_0^1(\Omega) \times \mathbb{R}$ with $\|u\|_{L^2(\Omega)} = 1$ such that, for any $\varphi \in H_0^1(\Omega)$, it holds that

$$(\nabla u, \nabla \varphi)_{L^2} + (Vu, \varphi)_{L^2} + \kappa(u^3, \varphi)_{L^2} = \lambda(u, \varphi)_{L^2}. \tag{4.1}$$

Recall that the eigenvalue associated with the ground state, referred to as the ground state eigenvalue, is the smallest among all eigenvalues of the problem.

Similarly, also any discrete ground state defined as the solution to the discrete constrained minimisation problem (2.4) satisfies the discrete eigenvalue problem: seek $(u_h, \lambda_h) \in \hat{U}_h \times \mathbb{R}$ with $\|u_{\mathcal{T}_h}\|_{L^2} = 1$ such that, for all $\hat{\varphi}_h \in \hat{U}_h$, it holds that

$$a_h(\hat{u}_h, \hat{\varphi}_h) + (Vu_{\mathcal{T}_h}, \varphi_{\mathcal{T}_h})_{L^2} + \kappa(u_{\mathcal{T}_h}^3, \varphi_{\mathcal{T}_h})_{L^2} = \lambda_h(u_{\mathcal{T}_h}, \varphi_{\mathcal{T}_h})_{L^2}, \tag{4.2}$$

where we recall the notation $\hat{u}_h = (u_{\mathcal{T}_h}, u_{\mathcal{F}_h})$ and analogously for the test function $\hat{\varphi}_h$. The discrete ground state eigenvalue λ_h is not necessarily the smallest among all discrete eigenvalues. As in the continuous setting, the discrete ground state energy and corresponding eigenvalue are related by $\lambda_h = 2E_h + \frac{\kappa}{2}\|u_{\mathcal{T}_h}\|_{L^4}^4$.

Remark 4.1 (Tilde notation). In the following, we will write $a \lesssim b$ or $b \gtrsim a$ if it holds that $a \leq Cb$ or $a \geq Cb$, respectively, where $C > 0$ is a constant that may depend on the domain, the mesh regularity, the coefficients V and κ, the ground state u, and the polynomial degree k, but is independent of the mesh size h.

Our first objective is to prove the plain convergence of the HHO method; precise convergence rates will be derived later.

Theorem 4.2 (Plain convergence of HHO method)**.** *As $h \to 0$, it holds that*

$$\|\nabla_h(\mathcal{R}_h\hat{u}_h - u)\|_{L^2} \to 0, \quad \|u - u_{\mathcal{T}_h}\|_{L^2} \to 0, \quad E_h \to E, \quad \lambda_h \to \lambda.$$

Proof. We begin by establishing the uniform boundedness of the discrete ground state energies E_h. Using definition (2.4), we directly obtain the estimate $E_h \leq \mathcal{E}_h(\mathcal{I}_h u / \|\Pi_{\mathcal{T}_h}^{k+1} u\|_{L^2})$. Its right-hand side can be bounded independently of h by an argument similar to that used in the proof of Theorem 3.1. Specifically, we apply Lemma A.2, (3.3), along with the uniform boundedness of $\mathcal{G}_h$ in the H^1-seminorm and of $\Pi_{\mathcal{T}_h}^{k+1}$ in the L^4-norm. Importantly, this bound is obtained without requiring any restriction on the stabilization parameter σ. As a direct consequence, we obtain the uniform boundedness of λ_h and $\|\hat{u}_h\|_{a_h}$, which in turn implies the uniform L^6-boundedness of $u_{\mathcal{T}_h}$ using Lemma A.3.

Consider the auxiliary Poisson problem, which seeks $u_h^c \in H_0^1(\Omega)$ such that

$$-\Delta u_h^c = -Vu_{\mathcal{T}_h} - \kappa u_{\mathcal{T}_h}^3 + \lambda_h u_{\mathcal{T}_h} =: f_h \tag{4.3}$$

holds in the weak sense. Since the L^2-norm of the right-hand side f_h is uniformly bounded, classical elliptic regularity results imply that $u_h^c \in H^2(\Omega) \cap H_0^1(\Omega)$, with H^2-norm uniformly bounded. Noting that $\hat{u}_h$ is the HHO approximation of the solution u_h^c to Poisson problem (4.3) with right-hand side f_h, classical approximation results for the HHO method (see, e.g., [DPD20, Thm. 2.27 & 2.28]) show that

$$\|\hat{u}_h - \mathcal{I}_h u_h^c\|_{a_h} + \|\nabla_h(\mathcal{R}_h\hat{u}_h - u_h^c)\|_{L^2} + |\hat{u}_h|_{s_h} \lesssim h. \tag{4.4}$$

From the latter estimate we can also derive the L^2-error estimate

$$\|u_{\mathcal{T}_h} - u_h^c\|_{L^2} \leq \|u_{\mathcal{T}_h} - \Pi_{\mathcal{T}_h}^{k+1} u_h^c\|_{L^2} + \|u_h^c - \Pi_{\mathcal{T}_h}^{k+1} u_h^c\|_{L^2} \lesssim h, \tag{4.5}$$

where we used Lemma A.3 and the approximation properties of $\Pi_{\mathcal{T}_h}^{k+1}$.

Next, we define an L^2-normalised version of u_h^c as $\tilde{u}_h^c := u_h^c / \|u_h^c\|_{L^2}$. Using the normalisation condition $\|u_{\mathcal{T}_h}\|_{L^2} = 1$ and (4.5), one can show that $|\|u_h^c\|_{L^2} - 1| \lesssim h$, so that the normalisation introduces only a perturbation of order h. Therefore, we can derive from (4.4) and (4.5) the estimate

$$\|\nabla_h(\mathcal{R}_h\hat{u}_h - \tilde{u}_h^c)\|_{L^2} + \|u_{\mathcal{T}_h} - \tilde{u}_h^c\|_{L^2} \lesssim h. \tag{4.6}$$

For the difference between E_h and $E_h^c \coloneqq \mathcal{E}(\tilde{u}_h^c)$ we obtain that

$$\begin{aligned} |E_h - E_h^c| &\leq \tfrac{1}{2}\left|(\nabla_h\mathcal{R}_h\hat{u}_h, \nabla_h\mathcal{R}_h\hat{u}_h)_{L^2} - (\nabla\tilde{u}_h^c, \nabla\tilde{u}_h^c)_{L^2}\right| + \tfrac{1}{2}\left|s_h(\hat{u}_h,\hat{u}_h)\right| \\ &+ \tfrac{1}{2}\left|(Vu_{\mathcal{T}_h}, u_{\mathcal{T}_h})_{L^2} - (V\tilde{u}_h^c, \tilde{u}_h^c)_{L^2}\right| + \tfrac{\kappa}{4}\left|(u_{\mathcal{T}_h}^3, u_{\mathcal{T}_h})_{L^2} - ((\tilde{u}_h^c)^3, \tilde{u}_h^c)_{L^2}\right| \lesssim h, \end{aligned} \tag{4.7}$$

where the last estimate follows from (4.4) and (4.6), the uniform L^6-boundedness of $u_{\mathcal{T}_h}$, and the uniform L^∞-boundedness of $\tilde{u}_h^c$. The latter is a consequence of the Sobolev embedding $H^2(\Omega) \hookrightarrow \mathcal{C}^0(\overline{\Omega})$ and the uniform H^2-boundedness of $\tilde{u}_h^c$.

Noting that $E_h - E \leq \mathcal{E}_h\left(\mathcal{I}_h u/\|u_{\mathcal{T}_h}\|_{L^2}\right) - E$, and proceeding similar as in the first part of this proof where we establish the uniform boundedness of E_h, we obtain that $E_h - E \lesssim h^2$. Together with $E \leq E_h^c$ and (4.7), this leads to

$$-h \lesssim E_h - E_h^c \leq E_h - E \lesssim h^2,$$

which directly implies that $E_h \to E$ as $h \to 0$. Using an argument similar to that in [CCM10, Thm. 1], one can further show that $\|u - \tilde{u}_h^c\|_{H^1} \to 0$. In combination with estimate (4.6), this implies the plain convergence results

$$\|u - u_{\mathcal{T}_h}\|_{L^2} \to 0, \quad \|\nabla_h(\mathcal{R}_h\hat{u}_h - u)\|_{L^2} \to 0. \tag{4.8}$$

From the first estimate in (4.8), we additionally obtain that

$$|\lambda - \lambda_h| \leq 2|E - E_h| + \tfrac{\kappa}{2}\left|\|u_{\mathcal{T}_h}\|_{L^4}^4 - \|u\|_{L^4}^4\right| \to 0,$$

using the uniform L^6-boundedness of $u_{\mathcal{T}_h}$, along with an L^∞-estimate for u. □

An important step in proving convergence rates is to write the ground state $u \in H_0^1(\Omega)$ as the weak solution to the auxiliary Poisson problem

$$-\Delta u = \lambda u - Vu - \kappa u^3 =: f, \tag{4.9}$$

with homogeneous Dirichlet boundary conditions on $\partial\Omega$. This allows us to construct a discrete ground state approximation by considering the HHO discretisation of problem (4.9). The latter seeks $\hat{v}_h = (v_{\mathcal{T}_h}, v_{\mathcal{F}_h}) \in \hat{U}_h$ such that, for all $\hat{\varphi}_h \in \hat{U}_h$,

$$a_h(\hat{v}_h, \hat{\varphi}_h) = (f, \varphi_{\mathcal{T}_h})_{L^2}, \tag{4.10}$$

and classical HHO theory shows optimal convergence rates for this approximation; see, e.g., [DPD20, Thm. 2.27 & 2.28]. We emphasise that this approximation is introduced solely for theoretical analysis and is not computed in practice. Since $\hat{v}_h$ is generally not L^2-normalised, we define its L^2-normalised counterpart by

$$\hat{w}_h \coloneqq \hat{v}_h / \|v_{\mathcal{T}_h}\|_{L^2}.$$

In the following convergence proof, we apply the triangle inequality to split the error into two components: the error between u and $\hat{w}_h$, and the error between $\hat{w}_h$ and $\hat{u}_h$. The first of these two errors is estimated in the lemma below. In what follows, we denote for any $s \in \mathbb{N}$ by $H^s(\mathcal{T}_h)$ the broken Sobolev space consisting of functions whose restriction to each element $T \in \mathcal{T}_h$ belongs to $H^s(T)$.

Lemma 4.3 (Bound of first term)**.** *Assume that, for some $0 \leq r \leq k$, it holds that $u \in H^{r+2}(\mathcal{T}_h)$. Then, we have the following approximation results:*

$$\|w_{\mathcal{T}_h} - u\|_{L^2} + \|\hat{w}_h - \mathcal{I}_h u\|_{a_h} + \|\nabla_h(\mathcal{R}_h\hat{w}_h - u)\|_{L^2} + |\hat{w}_h|_{s_h} \lesssim h^{r+1}. \tag{4.11}$$

Proof. Applying classical HHO theory (see, e.g., [DPD20, Thm. 2.27 & 2.28]), yields an error estimate of the form (4.11) for the HHO approximation $\hat{v}_h$. To transfer this estimate to its L^2-normalised counterpart $\hat{w}_h$, we observe that

$$\|v_{\mathcal{T}_h} - u\|_{L^2} \leq \|v_{\mathcal{T}_h} - \Pi_{\mathcal{T}_h}^{k+1} u\|_{L^2} + \|\Pi_{\mathcal{T}_h}^{k+1} u - u\|_{L^2} \lesssim h^{r+1},$$

where we used Lemma A.3 along with the approximation properties of $\Pi_{\mathcal{T}_h}^{k+1}$. Due to the L^2-normalization condition $\|u\|_{L^2} = 1$, it follows that $|\|v_{\mathcal{T}_h}\|_{L^2} - 1| \lesssim h^{r+1}$, which readily implies the assertion. □

It remains to bound the second error, which is done in the following lemma.

Lemma 4.4 (Bound of second term)**.** *Assume that, for some* $0 \leq r \leq k$*, it holds that* $u \in H^{r+2}(\mathcal{T}_h)$*. Then, we have the following estimate:*

$$\begin{aligned}\|u_{\mathcal{T}_h} - w_{\mathcal{T}_h}\|_{L^2} + \|\nabla_h \mathcal{R}_h(\hat{u}_h - \hat{w}_h)\|_{L^2} + |\hat{u}_h|_{s_h} + |\hat{u}_h - \hat{w}_h|_{s_h} \\ \lesssim \|(u_{\mathcal{T}_h} - u)^2\|_{L^3} + h\|u_{\mathcal{T}_h} - u\|_{L^2} + h|\lambda_h - \lambda| + h^{r+1}.\end{aligned}$$

Proof. In this proof, we write pairs of functions in $L^2(\Omega) \times H^1(\mathcal{T}_h)$ in Roman boldface letters, e.g., $\mathbf{u}$, $\mathbf{v}$, and $\mathbf{w}$. Given the ground state u and the corresponding eigenvalue λ, we define the bilinear form $J_{u,\lambda}$ for any $\mathbf{v} = (v, \gamma)$ and $\mathbf{w} = (w, \tau)$ as

$$J_{u,\lambda}(\mathbf{v}, \mathbf{w}) := (\nabla_h \gamma, \nabla_h \tau)_\Omega + (Vv, w)_\Omega + 3\kappa(|u|^2 v, w)_\Omega - \lambda(v, w)_\Omega.$$

Further, denote $\mathbf{u}_h := (u_{\mathcal{T}_h}, \mathcal{R}_h \hat{u}_h)$ and $\mathbf{w}_h := (w_{\mathcal{T}_h}, \mathcal{R}_h \hat{w}_h)$, and abbreviate $\mathbf{y}_h := \mathbf{u}_h - \mathbf{w}_h$ and $\hat{y}_h := \hat{u}_h - \hat{w}_h$. The function $\hat{y}_h$ can be seen as the HHO approximation to the weak solution of the auxiliary Poisson problem: seek $\chi \in H_0^1(\Omega)$ such that

$$-\Delta\chi = f_h - f/\|v_{\mathcal{T}_h}\|_{L^2} =: g_h$$

with f and f_h defined in (4.9) and (4.3), respectively. By classical elliptic regularity, $\chi \in H^2(\Omega) \cap H_0^1(\Omega)$ with $\|\chi\|_{H^2} \lesssim \|g_h\|_{L^2} \lesssim 1$, since g_h is uniformly L^2-bounded. Applying classical HHO convergence results for the Poisson problem (see, e.g., [DPD20, Thm. 2.27 & 2.28]) along with Lemma A.3, we obtain that

$$\|y_{\mathcal{T}_h} - \chi\|_{L^2} + \|\nabla_h(\mathcal{R}_h \hat{y}_h - \chi)\|_{L^2} \lesssim h\|\chi\|_{H^2}. \tag{4.12}$$

To estimate the discrete errors associated with $\hat{y}_h$, we use the identity

$$\|y_{\mathcal{T}_h}\|_{L^2}^2 = \|\chi\|_{L^2}^2 + (y_{\mathcal{T}_h} - \chi, y_{\mathcal{T}_h} + \chi)_{L^2},$$

and a similar one for the term $\|\nabla_h \mathcal{R}_h \hat{y}_h\|_{L^2}^2$. Applying (4.12) and the weighted Young's inequality with parameter $\epsilon > 0$, this leads to the estimate

$$\begin{aligned}&\|y_{\mathcal{T}_h}\|_{L^2}^2 + \|\nabla_h \mathcal{R}_h \hat{y}_h\|_{L^2}^2 \\ &\lesssim \|\chi\|_{L^2}^2 + \|\nabla\chi\|_{L^2}^2 + h\|\chi\|_{H^2}(h\|\chi\|_{H^2} + \|y_{\mathcal{T}_h}\|_{L^2} + \|\nabla_h \mathcal{R}_h \hat{y}_h\|_{L^2}) \\ &\leq \|\chi\|_{L^2}^2 + \|\nabla\chi\|_{L^2}^2 + (1 + \tfrac{1}{4\epsilon})h^2\|\chi\|_{H^2}^2 + \epsilon(\|y_{\mathcal{T}_h}\|_{L^2}^2 + \|\nabla_h \mathcal{R}_h \hat{y}_h\|_{L^2}^2).\end{aligned} \tag{4.13}$$

Choosing the parameter ϵ sufficiently small (independently of h) allows the last term on the right-hand side to be absorbed into the left-hand side, yielding

$$\|y_{\mathcal{T}_h}\|_{L^2}^2 + \|\nabla_h \mathcal{R}_h \hat{y}_h\|_{L^2}^2 \lesssim \|\chi\|_{L^2}^2 + \|\nabla\chi\|_{L^2}^2 + h^2\|\chi\|_{H^2}^2 \lesssim J_{u,\lambda}(\mathbf{x}, \mathbf{x}) + h^2\|\chi\|_{H^2}^2,$$

where the second estimate follows from [CCM10, Lem. 1] with $\mathbf{x} := (\chi, \chi)$. The referenced result applies only in the conforming setting, and thus for the pair $\mathbf{x}$, but not directly for its discrete counterpart $\mathbf{y}_h$. To relate back to $\mathbf{y}_h$, we invoke estimate (4.12), the L^∞-bound for u, and the weighted Young's inequality with parameter $\delta > 0$. Proceeding similarly to estimate (4.13), we obtain

$$|J_{u,\lambda}(\mathbf{y}_h, \mathbf{y}_h) - J_{u,\lambda}(\mathbf{x}, \mathbf{x})| \lesssim \left(1 + \tfrac{1}{4\delta}\right) h^2\|\chi\|_{H^2}^2 + \delta\left(\|y_{\mathcal{T}_h}\|_{L^2}^2 + \|\nabla_h \mathcal{R}_h \hat{y}_h\|_{L^2}^2\right).$$

Combining this with the previous estimate and choosing δ sufficiently small (independent of h) allows to absorb the last term into the left-hand side, yielding

$$\begin{aligned}\|y_{\mathcal{T}_h}\|_{L^2}^2 + \|\nabla_h \mathcal{R}_h \hat{y}_h\|_{L^2}^2 &\lesssim J_{u,\lambda}(\mathbf{y}_h, \mathbf{y}_h) + h^2\|\chi\|_{H^2}^2 \\ &= \underbrace{J_{u,\lambda}(\mathbf{u}_h - \mathbf{u}, \mathbf{y}_h)}_{=:\Xi_1} + \underbrace{J_{u,\lambda}(\mathbf{u} - \mathbf{w}_h, \mathbf{y}_h)}_{=:\Xi_2} + \underbrace{h^2\|\chi\|_{H^2}^2}_{=:\Xi_3},\end{aligned} \tag{4.14}$$

where we denote $\mathbf{u} \coloneqq (u, u)$.

To prepare the estimate for Ξ_1, we observe the following identity:

$$J_{u,\lambda}(\mathbf{u}_h, \mathbf{y}_h) = (\lambda_h - \lambda)(u_{\mathcal{T}_h}, y_{\mathcal{T}_h})_{L^2} + \kappa(3u^2 u_{\mathcal{T}_h} - u_{\mathcal{T}_h}^3, y_{\mathcal{T}_h})_{L^2} - s_h(\hat{u}_h, \hat{y}_h),$$

where we added and subtracted the terms $s_h(\hat{u}_h, \hat{y}_h)$ and $\kappa(u_{\mathcal{T}_h}^2, y_{\mathcal{T}_h})_{L^2}$, and applied (4.2) with the test function $\hat{y}_h$. Furthermore, we have the identity

$$J_{u,\lambda}(\mathbf{u}, \mathbf{y}_h) = (\nabla u, \nabla_h(\mathcal{R}_h\hat{y}_h - \mathcal{J}_h\hat{y}_h))_{L^2} + (\Delta u, y_{\mathcal{T}_h} - \mathcal{J}_h\hat{y}_h)_{L^2} + \kappa(2u^3, y_{\mathcal{T}_h})_{L^2},$$

where we added and subtracted terms involving the moment-preserving smoother $\mathcal{J}_h \colon \hat{U}_h \to H_0^1(\Omega)$ from Lemma A.4, allowing us to apply (4.1) with $\mathcal{J}_h\hat{y}_h$ as test function, and we used the identity $Vu + \kappa u^3 - \lambda u = \Delta u$. Combining the two identities above and noting that

$$(u_{\mathcal{T}_h}, y_{\mathcal{T}_h})_{L^2} = \tfrac{1}{2}\|u_{\mathcal{T}_h} - w_{\mathcal{T}_h}\|_{L^2}^2, \quad s_h(\hat{u}_h, \hat{y}_h) = \tfrac{1}{2}\big(|\hat{u}_h|_{s_h}^2 + |\hat{u}_h - \hat{w}_h|_{s_h}^2 - |\hat{w}_h|_{s_h}^2\big),$$

where the first relation follows from the fact that $\|u_{\mathcal{T}_h}\|_{L^2} = \|w_{\mathcal{T}_h}\|_{L^2}$, yields that

$$\begin{aligned}\Xi_1 = &-\kappa((u - u_{\mathcal{T}_h})^2(2u + u_{\mathcal{T}_h}), y_{\mathcal{T}_h})_{L^2} - \tfrac{1}{2}(|\hat{u}_h|_{s_h}^2 + |\hat{y}_h|_{s_h}^2 - |\hat{w}_h|_{s_h}^2) \\ &+ \tfrac{1}{2}(\lambda_h - \lambda)\|y_{\mathcal{T}_h}\|_{L^2}^2 - (\nabla u, \nabla_h(\mathcal{R}_h\hat{y}_h - \mathcal{J}_h\hat{y}_h))_{L^2} - (\Delta u, y_{\mathcal{T}_h} - \mathcal{J}_h\hat{y}_h)_{L^2}.\end{aligned}$$

Next, we reformulate inequality (4.14) with the help of the latter identity, where we move the terms $|\hat{u}_h|_{s_h}^2$ and $|\hat{y}_h|_{s_h}^2$ to the left-hand side. This gives that

$$\begin{aligned}&\|y_{\mathcal{T}_h}\|_{L^2}^2 + \|\nabla_h\mathcal{R}_h\hat{y}_h\|_{L^2}^2 + |\hat{u}_h|_{s_h}^2 + |\hat{y}_h|_{s_h}^2 \\ &\quad\lesssim |((u - u_{\mathcal{T}_h})^2(2u + u_{\mathcal{T}_h}), y_{\mathcal{T}_h})_{L^2}| + |\hat{w}_h|_{s_h}^2 + |\lambda_h - \lambda|\|y_{\mathcal{T}_h}\|_{L^2}^2 \\ &\qquad + |(\nabla u, \nabla_h(\mathcal{R}_h\hat{y}_h - \mathcal{J}_h\hat{y}_h))_{L^2}| + |(\Delta u, y_{\mathcal{T}_h} - \mathcal{J}_h\hat{y}_h)_{L^2}| + |\Xi_2| + |\Xi_3|.\end{aligned} \tag{4.15}$$

In the following, we estimate the terms on the right-hand side individually. For the first term, the uniform L^6-boundedness of both u and $u_{\mathcal{T}_h}$ implies that

$$|((u - u_{\mathcal{T}_h})^2(2u + u_{\mathcal{T}_h}), y_{\mathcal{T}_h})_{L^2}| \lesssim \|(u - u_{\mathcal{T}_h})^2\|_{L^3}\|y_{\mathcal{T}_h}\|_{L^2}.$$

The second term on the right-hand side of (4.15) is estimated using Lemma 4.3, while the third term can be absorbed into the left-hand side for h sufficiently small.

Using the properties of $\mathcal{J}_h$ from Lemma A.4, we estimate the next two terms as

$$\begin{aligned}|(\nabla u, \nabla_h(\mathcal{R}_h\hat{y}_h - \mathcal{J}_h\hat{y}_h))_{L^2}| &= |(\nabla_h(u - \mathcal{G}_h u), \nabla_h\mathcal{J}_h\hat{y}_h)_{L^2}| \lesssim h^{r+1}\|\hat{y}_h\|_{a_h}, \\ |(\Delta u, y_{\mathcal{T}_h} - \mathcal{J}_h\hat{y}_h)_{L^2}| &= |(h(\mathtt{id} - \Pi_{\mathcal{T}_h}^{k+1})\Delta u, h^{-1}(y_{\mathcal{T}_h} - \mathcal{J}_h\hat{y}_h))_{L^1}| \lesssim h^{r+1}\|\hat{y}_h\|_{a_h},\end{aligned}$$

where, for the latter estimate, we used that $u \in H^{r+2}(\mathcal{T}_h)$, which implies that $\Delta u \in H^r(\mathcal{T}_h)$, in combination with the estimate

$$\|h^{-1}(y_{\mathcal{T}_h} - \mathcal{J}_h\hat{y}_h)\|_{L^2} = \|h^{-1}(\mathtt{id} - \Pi_{\mathcal{T}_h}^{k+1})\mathcal{J}_h\hat{y}_h\|_{L^2} \lesssim \|\hat{y}_h\|_{a_h},$$

by the approximation properties of $\Pi_{\mathcal{T}_h}^{k+1}$.

Therefore, it only remains to estimate Ξ_2 and Ξ_3. From the continuity of the bilinear form $J_{u,\lambda}$ and Lemma 4.3, we obtain for Ξ_2 that

$$|\Xi_2| \lesssim h^{r+1}(\|y_{\mathcal{T}_h}\|_{L^2} + \|\nabla_h\mathcal{R}_h\hat{y}_h\|_{L^2}).$$

Finally, the term Ξ_3 can be estimated as

$$|\Xi_3| \lesssim h^2\|f_h - f/\|v_{\mathcal{T}_h}\|_{L^2}\|_{L^2}^2 \lesssim h^2\|u_{\mathcal{T}_h} - u\|_{L^2}^2 + h^2|\lambda_h - \lambda|^2 + h^{2r+4},$$

where f and f_h are defined in (4.9) and (4.3), respectively. Here, we used that $|1-\|v_{\mathcal{T}_h}\|_{L^2}| \lesssim h^{r+1}$, as shown in the proof of Lemma 4.3, and that both u and $u_{\mathcal{T}_h}$ are uniformly L^4-bounded.

Combining the above estimates, we obtain

$$\begin{aligned}\|y_{\mathcal{T}_h}\|_{L^2}^2 &+ \|\nabla_h \mathcal{R}_h \hat{y}_h\|_{L^2}^2 + |\hat{u}_h|_{s_h}^2 + |\hat{y}_h|_{s_h}^2 \\ &\lesssim h^{r+1}(\|\hat{y}_h\|_{a_h} + \|y_{\mathcal{T}_h}\|_{L^2}) + \|(u-u_{\mathcal{T}_h})^2\|_{L^3}\|y_{\mathcal{T}_h}\|_{L^2} \\ &\quad + h^2\|u_{\mathcal{T}_h} - u\|_{L^2}^2 + h^2|\lambda_h - \lambda|^2 + h^{2r+2} + h^{2r+4},\end{aligned}$$

and the assertion can be concluded using the weighted Young's inequality. □

The following theorem gives a convergence result for the ground state, energy, and eigenvalue approximations of the proposed HHO method.

Theorem 4.5 (A priori error estimate)**.** *Assume that $u \in H^{r+2}(\mathcal{T}_h)$ for some $0 \le r \le k$. Then, the following approximation results hold for the ground state:*

$$\|u_{\mathcal{T}_h} - u\|_{L^2} + \|\nabla_h(\mathcal{R}_h\hat{u}_h - u)\|_{L^2} + |\hat{u}_h|_{s_h} + |\hat{u}_h - \mathcal{I}_h u|_{s_h} \lesssim h^{r+1}. \tag{4.16}$$

The eigenvalue and energy approximations further satisfy

$$|\lambda - \lambda_h| \lesssim h^{r+1}, \quad |E - E_h| \lesssim h^{2r+2}. \tag{4.17}$$

Proof. Using the triangle inequality and Lemmas 4.3 and 4.4, we obtain

$$\begin{aligned}\|u_{\mathcal{T}_h} - u\|_{L^2} &+ \|\nabla_h(\mathcal{R}_h\hat{u}_h - u)\|_{L^2} + |\hat{u}_h|_{s_h} + |\hat{u}_h - \mathcal{I}_h u|_{s_h} \\ &\lesssim h^{r+1} + \|(u-u_{\mathcal{T}_h})^2\|_{L^3} + h\|u_{\mathcal{T}_h} - u\|_{L^2} + h|\lambda_h - \lambda|.\end{aligned} \tag{4.18}$$

In the following, we consider the terms on the right-hand side of the latter inequality individually. For the second term, we obtain with the triangle inequality that

$$\|(u-u_{\mathcal{T}_h})^2\|_{L^3} \lesssim \|u - \Pi_{\mathcal{T}_h}^{k+1}u\|_{L^6}^2 + \|\Pi_{\mathcal{T}_h}^{k+1}u - u_{\mathcal{T}_h}\|_{L^6}^2, \tag{4.19}$$

where the first term can estimated using classical approximation results for the L^2-projection $\Pi_{\mathcal{T}_h}^{k+1}$ in the L^6-norm, as well as the (broken) Sobolev embedding $W^{r+1,6}(\mathcal{T}_h) \hookrightarrow H^{r+2}(\mathcal{T}_h)$ to obtain that

$$\|u - \Pi_{\mathcal{T}_h}^{k+1}u\|_{L^6} \lesssim h^{r+1}|u|_{W^{r+1,6}(\mathcal{T}_h)} \lesssim h^{r+1}\|u\|_{H^{r+2}(\mathcal{T}_h)}$$

For the second term on the right-hand side of (4.19), we use the discrete Sobolev embedding from Lemma A.3, the triangle inequality, (3.3), and the approximation properties of the Galerkin projection to get that

$$\begin{aligned}\|\Pi_{\mathcal{T}_h}^{k+1}u - u_{\mathcal{T}_h}\|_{L^6}^2 &\lesssim \|\hat{u}_h - \mathcal{I}_h u\|_{a_h}^2 \\ &\lesssim \|\nabla_h(\mathcal{R}_h\hat{u}_h - u)\|_{L^2}^2 + \|\nabla_h(u - \mathcal{G}_h u)\|_{L^2}^2 + |\hat{u}_h - \mathcal{I}_h u|_{s_h}^2 \\ &\lesssim h^{2r+2} + \|\nabla_h(\mathcal{R}_h\hat{u}_h - u)\|_{L^2}^2 + |\hat{u}_h - \mathcal{I}_h u|_{s_h}^2.\end{aligned}$$

Using the latter two estimates we can continue (4.19) as

$$\|(u-u_{\mathcal{T}_h})^2\|_{L^3} \lesssim h^{2r+2} + \|\nabla_h(\mathcal{R}_h\hat{u}_h - u)\|_{L^2}^2 + |\hat{u}_h - \mathcal{I}_h u|_{s_h}^2. \tag{4.20}$$

Thanks to the plain convergence result of Theorem 4.2, $\|(u-u_{\mathcal{T}_h})^2\|_{L^3}$ is a higher-order term, and can thus be absorbed in the left-hand side for sufficiently small $h > 0$. Note that, similarly, also the third term on the right-hand side of (4.18) can be absorbed into the left-hand side, for $h > 0$ sufficiently small.

To estimate the fourth term on the right-hand side of (4.18), we note that

$$|\lambda - \lambda_h| \lesssim \|u_{\mathcal{T}_h} - u\|_{L^2} + \|\nabla_h(\mathcal{R}_h\hat{u}_h - u)\|_{L^2} + |\hat{u}_h|_{s_h}^2, \tag{4.21}$$

where we have used that $\|\hat{u}_h\|_{a_h}$ and $\|u_{\mathcal{T}_h}\|_{L^6}$ are uniformly bounded. Therefore, this term is also of higher order and can be absorbed into the left-hand term for sufficiently small $h > 0$. Convergence result (4.16) follows from combining the above estimates. The first estimate in (4.17), which is the desired eigenvalue approximation result, follows by combining (4.16) and (4.21).

Finally, for proving the desired energy approximation result, we note that

$$E - E_h = \tfrac{1}{2}\|\nabla_h(u - \mathcal{R}_h\hat{u}_h)\|_{L^2}^2 + \tfrac{1}{2}\|V^{1/2}(u - u_{\mathcal{T}_h})\|_{L^2}^2 - \tfrac{1}{2}|\hat{u}_h|_{s_h}^2 + R,$$

where the first and second terms on the right-hand side are of order $2r+2$, using (4.16). In what follows, we will also show that the remainder R, defined as

$$R \coloneqq (\nabla_h(u - \mathcal{R}_h\hat{u}_h), \nabla_h\mathcal{R}_h\hat{u}_h)_{L^2} + (V(u - u_{\mathcal{T}_h}), u_{\mathcal{T}_h})_{L^2} + \tfrac{1}{4}\kappa(\|u\|_{L^4}^4 - \|u_{\mathcal{T}_h}\|_{L^4}^4)$$

is of order $2r+2$. To this end, we first rewrite the remainder R, using (4.2) with the test function $\mathcal{I}_h u - \hat{u}_h$, the identity $(\Pi_{\mathcal{T}_h}^{k+1}u - u_{\mathcal{T}_h}, u_{\mathcal{T}_h})_{L^2} = -\frac{1}{2}\|u - u_{\mathcal{T}_h}\|_{L^2}^2$, and some further algebraic manipulations, to obtain that

$$\begin{aligned} R &= \lambda_h(\Pi_{\mathcal{T}_h}^{k+1}u - u_{\mathcal{T}_h}, u_{\mathcal{T}_h})_{L^2} - \kappa(u_{\mathcal{T}_h}^3, \Pi_{\mathcal{T}_h}^{k+1}u - u_{\mathcal{T}_h})_{L^2} + \tfrac{1}{4}\kappa(\|u\|_{L^4}^4 - \|u_{\mathcal{T}_h}\|_{L^4}^4) \\ &\quad - s_h(\hat{u}_h, \mathcal{I}_h u - \hat{u}_h) + (V(u - \Pi_{\mathcal{T}_h}^{k+1}u), u_{\mathcal{T}_h})_{L^2} \\ &= -\tfrac{1}{2}\lambda_h\|u - u_{\mathcal{T}_h}\|_{L^2}^2 + \tfrac{\kappa}{4}((u_{\mathcal{T}_h} - u)^2, 3u_{\mathcal{T}_h}^2 + 2u_{\mathcal{T}_h}u + u^2)_{L^2} \\ &\quad - s_h(\hat{u}_h, \mathcal{I}_h u - \hat{u}_h) + (u - \Pi_{\mathcal{T}_h}^{k+1}u, V u_{\mathcal{T}_h} + \kappa u_{\mathcal{T}_h}^3)_{L^2}. \end{aligned}$$

Using Lemma 4.4 and (4.16), it directly follows that all terms except the last one are of order $2r+2$. To show that also the last term is of this order, we observe that

$$\begin{aligned} &(\kappa u_{\mathcal{T}_h}^3 + V u_{\mathcal{T}_h}, u - \Pi_{\mathcal{T}_h}^{k+1}u)_{L^2} \\ &\quad = (\Delta u + \lambda u, u - \Pi_{\mathcal{T}_h}^{k+1}u)_{L^2} + (\kappa u_{\mathcal{T}_h}^3 + V u_{\mathcal{T}_h} - \kappa u^3 - V u, u - \Pi_{\mathcal{T}_h}^{k+1}u)_{L^2}, \end{aligned} \tag{4.22}$$

where we have used (4.9). Since, by assumption, $u \in H^{r+2}(\mathcal{T}_h)$, it follows that $\Delta u \in H^r(\mathcal{T}_h)$, allowing us to apply the orthogonality and approximation properties of $\Pi_{\mathcal{T}_h}^{k+1}$ to show that the first term is of order $2r+2$. A similar bound for the second term is obtained directly from (4.16). Consequently, all terms in (4.22) are of order $2r+2$, and the energy approximation estimate in (4.17) follows. ☐

The L^2- and eigenvalue approximation estimates stated in (4.16) and (4.17) can be improved as outlined in the following theorem.

Theorem 4.6 (Improved error estimate)**.** *Assume that $u \in H^{r+2}(\mathcal{T}_h)$ for some $0 \le r \le k$. Then, the following L^2-approximation results hold for the ground state:*

$$\|u_{\mathcal{T}_h} - u\|_{L^2} + \|\mathcal{R}_h\hat{u}_h - u\|_{L^2} \lesssim h^{r+2}. \tag{4.23}$$

Furthermore, we can improve the eigenvalue approximation estimate to

$$|\lambda - \lambda_h| \lesssim h^{r+2}. \tag{4.24}$$

Proof. We begin by introducing an auxiliary problem. For any given $w \in L^2(\Omega)$, it seeks $\psi_w \in H_0^1(\Omega)$ such that the following equation holds in the weak sense:

$$-\Delta\psi_w + (V + 3\kappa u^2 - \lambda)\psi_w = 2\kappa(u^3, \psi_w)_\Omega\, u + w - (w, u)_\Omega\, u.$$

It can be verified that this problem is solved by the unique solution $\psi_w \in u^\perp := \{v \in H_0^1(\Omega) : (u, v)_\Omega = 0\}$ satisfying, for all $v \in u^\perp$, the variational problem

$$(\nabla\psi_w, \nabla v)_{L^2} + ((V + 3\kappa u^2 - \lambda)\psi_w, v)_{L^2} = (w, v)_{L^2}. \tag{4.25}$$

The well-posedness of the latter problem follows from the Lax–Milgram theorem using the coercivity of the bilinear form on the left-hand side (cf. [CCM10, Lem. 1]) and the fact that $u^\perp$ is a closed subspace of $H_0^1(\Omega)$. Classical elliptic regularity then gives that $\psi_w \in H^2(\Omega) \cap H_0^1(\Omega)$ with the estimate $\|\psi_w\|_{H^2} \lesssim \|w\|_{L^2}$.

Next, we define the error $\hat{e}_h = (e_{\mathcal{T}h}, e_{\mathcal{F}_h}) := \hat{u}_h - \mathcal{I}_h u$, test equation (4.25) with the function $\mathcal{J}_h\hat{e}_h - (\mathcal{J}_h\hat{e}_h, u)_{L^2} u \in u^\perp$, where $\mathcal{J}_h$ denotes the moment preserving operator from Lemma A.4, and set $w := e_{\mathcal{T}_h}$. This yields that

$$
\begin{aligned}
\|e_{\mathcal{T}_h}\|_{L^2}^2 &= (e_{\mathcal{T}_h}, \mathcal{J}_h\hat{e}_h - (\mathcal{J}_h\hat{e}_h, u)_{L^2}\, u)_{L^2} + (\mathcal{J}_h\hat{e}_h, u)_{L^2}\,(e_{\mathcal{T}_h}, u)_{L^2} \\
&= \underbrace{(\nabla\psi_{e_{\mathcal{T}_h}}, \nabla\mathcal{J}_h\hat{e}_h)_{L^2} + ((V + 3\kappa u^2 - \lambda)\,\psi_{e_{\mathcal{T}_h}}, \mathcal{J}_h\hat{e}_h)_{L^2}}_{=:\Xi_1} \\
&\qquad - \underbrace{(\mathcal{J}_h\hat{e}_h, u)_{L^2}\big((\nabla\psi_{e_{\mathcal{T}_h}}, \nabla u)_{L^2} + ((V + 3\kappa u^2 - \lambda)\,\psi_{e_{\mathcal{T}_h}}, u)_{L^2}\big)}_{=:\Xi_2} \\
&\qquad + \underbrace{(\mathcal{J}_h\hat{e}_h, u)_{L^2}\,(e_{\mathcal{T}_h}, u)_{L^2}}_{=:\Xi_3}.
\end{aligned}
$$

Before estimating terms Ξ_1–Ξ_3, we first derive a bound for $|(\mathcal{J}_h\hat{e}_h, u)_{L^2}|$. To this end, we use the properties of $\mathcal{J}_h$ as stated in Lemma A.4, which yields that

$$
(\mathcal{J}_h\hat{e}_h, u)_{L^2} = (e_{\mathcal{T}_h}, u_{\mathcal{T}_h})_{L^2} + (\mathcal{J}_h\hat{e}_h, u - u_{\mathcal{T}_h})_{L^2}. \tag{4.26}
$$

The two terms on the right-hand side can be individually estimated as

$$
\begin{aligned}
|(e_{\mathcal{T}_h}, u_{\mathcal{T}_h})_{L^2}| &= |(u_{\mathcal{T}_h} - u, u_{\mathcal{T}_h})_{L^2}| = \tfrac{1}{2}\|u - u_{\mathcal{T}_h}\|_{L^2}^2 \lesssim h^{2r+2}, \\
|(\mathcal{J}_h\hat{e}_h, u - u_{\mathcal{T}_h})_{L^2}| &\le \|\mathcal{J}_h\hat{e}_h\|_{L^2}\|u - u_{\mathcal{T}_h}\|_{L^2} \lesssim \|\hat{e}_h\|_{a_h}\|u - u_{\mathcal{T}_h}\|_{L^2} \lesssim h^{2r+2},
\end{aligned}
$$

where we used the H^1-continuity of $\mathcal{J}_h$ and the error estimates provided in Theorem 4.5. By inserting the latter two bounds into (4.26), we obtain that

$$
|(\mathcal{J}_h\hat{e}_h, u)_{L^2}| \lesssim h^{2r+2}.
$$

Combining this estimate with the L^∞-bound for u and recalling the H^2-regularity estimate $\|\psi_{e_{\mathcal{T}_h}}\|_{H^2} \lesssim \|e_{\mathcal{T}_h}\|_{L^2}$, we obtain the following bounds for Ξ_2 and Ξ_3:

$$
|\Xi_2| \lesssim h^{2r+2}\|\psi_{e_{\mathcal{T}_h}}\|_{H^1} \lesssim h^{2r+2}\|e_{\mathcal{T}_h}\|_{L^2}, \qquad |\Xi_3| \lesssim h^{2r+2}\|e_{\mathcal{T}_h}\|_{L^2}.
$$

For estimating term Ξ_1, we introduce the function

$$
\hat{\phi}_h = (\phi_{\mathcal{T}_h}, \phi_{\mathcal{F}_h}) := \mathcal{I}_h\left(\psi_{e_{\mathcal{T}_h}} - \frac{(\psi_{e_{\mathcal{T}_h}}, \Pi_{\mathcal{T}_h}^{k+1}u)_{L^2}}{(u, \Pi_{\mathcal{T}_h}^{k+1}u)_{L^2}}u\right) \in \hat{U}_h,
$$

for which, by construction, it holds that $(\phi_{\mathcal{T}_h}, u)_{L^2} = 0$. To estimate terms involving $\hat{\phi}_h$, the following bounds will play an important role:

$$
|(\psi_{e_{\mathcal{T}_h}}, \Pi_{\mathcal{T}_h}^{k+1}u)_{L^2}| = |(\psi_{e_{\mathcal{T}_h}} - \Pi_{\mathcal{T}_h}^{1}\psi_{e_{\mathcal{T}_h}}, \Pi_{\mathcal{T}_h}^{k+1}u - u)_{L^2}| \lesssim h^{r+4}\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}, \tag{4.27}
$$

$$
|(u, \Pi_{\mathcal{T}_h}^{k+1}u)_{L^2}| = |(\Pi_{\mathcal{T}_h}^{k+1}u, \Pi_{\mathcal{T}_h}^{k+1}u)_{L^2}| = |1 - \|u - \Pi_{\mathcal{T}_h}^{k+1}u\|_{L^2}^2| \gtrsim 1 - \tfrac{h^4}{\pi^4}. \tag{4.28}
$$

The proof of these bounds relies on the fact that $\psi_{e_{\mathcal{T}_h}} \in u^\perp$, together with the approximation and orthogonality properties of $\Pi_{\mathcal{T}_h}^{k+1}$ and the Pythagorean identity. Direct calculations based on (4.27) and (4.28), which are omitted here for the sake of brevity, then yield the following approximation results:

$$
\|\nabla_h(\psi_{e_{\mathcal{T}_h}} - \mathcal{R}_h\hat{\phi}_h)\|_{L^2} + \|\nabla(\mathcal{J}_h\hat{\phi}_h - \psi_{e_{\mathcal{T}_h}})\|_{L^2} + |\phi_h|_{s_h} \lesssim h\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}, \tag{4.29}
$$

$$
\|\psi_{e_{\mathcal{T}_h}} - \phi_{\mathcal{T}_h}\|_{L^2} + \|\mathcal{J}_h\hat{\phi}_h - \psi_{e_{\mathcal{T}_h}}\|_{L^2} \lesssim h^2\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}. \tag{4.30}
$$

To estimate the term Ξ_1, we start by rewriting it as

$$
\begin{aligned}
\Xi_1 &= (\nabla\mathcal{J}_h\hat{e}_h, \nabla_h\mathcal{R}_h\hat{\phi}_h)_{L^2} + ((V + 3\kappa u^2 - \lambda)\mathcal{J}_h\hat{e}_h, \phi_{\mathcal{T}_h})_{L^2} \\
&\qquad + (\nabla\mathcal{J}_h\hat{e}_h, \nabla\psi_{e_{\mathcal{T}_h}} - \nabla_h\mathcal{R}_h\hat{\phi}_h)_{L^2} + ((V + 3\kappa u^2 - \lambda)\mathcal{J}_h\hat{e}_h, \psi_{e_{\mathcal{T}_h}} - \phi_{\mathcal{T}_h})_{L^2}.
\end{aligned} \tag{4.31}
$$

Using the properties of $\mathcal{J}_h$ from Lemma A.4, together with (4.1) and (4.2) and some algebraic manipulations, we arrive at the identity

$$
\begin{aligned}
&(\nabla \mathcal{J}_h \hat{e}_h, \nabla_h \mathcal{R}_h \hat{\phi}_h)_{L^2} + ((V + 3\kappa u^2 - \lambda)\mathcal{J}_h \hat{e}_h, \phi_{\mathcal{T}_h})_{L^2} \\
&\quad = \underbrace{((3\kappa u^2 - \kappa u_{\mathcal{T}_h}^2 + \lambda_h - \lambda)u_{\mathcal{T}_h}, \phi_{\mathcal{T}_h})_{L^2} - (2\kappa u^3, \phi_{\mathcal{T}_h})_{L^2}}_{=:\xi_1} - \underbrace{s_h(\phi_h, \hat{u}_h)}_{=:\xi_2} \\
&\qquad + \underbrace{(\nabla_h(u - \mathcal{G}_h u), \nabla \mathcal{J}_h \hat{\phi}_h)_{L^2}}_{=:\xi_3} + \underbrace{((V + \kappa u^2 - \lambda)u, \mathcal{J}_h \hat{\phi}_h - \phi_{\mathcal{T}_h})_{L^2}}_{=:\xi_4} \\
&\qquad + \underbrace{((V + 3\kappa u^2 - \lambda)(\mathcal{J}_h \hat{e}_h - e_{\mathcal{T}_h}), \phi_{\mathcal{T}_h})_{L^2}}_{=:\xi_5} \\
&\qquad + \underbrace{((V + 3\kappa u^2 - \lambda)(u - \Pi_{\mathcal{T}_h}^{k+1} u), \phi_{\mathcal{T}_h})_{L^2}}_{=:\xi_6},
\end{aligned}
$$

where terms ξ_1–ξ_6 are estimated individually in the following.

Using Theorem 4.5, (4.29) and (4.30), the approximation properties of the Galerkin- and L^2-projections, and the properties of $\mathcal{J}_h$ from Lemma A.4, we obtain that

$$
\begin{aligned}
|\xi_1| &\leq |\kappa((u - u_{\mathcal{T}_h})^2(2u + u_{\mathcal{T}_h}), \phi_{\mathcal{T}_h})_{L^2}| \\
&\qquad + |\lambda_h - \lambda||(u - u_{\mathcal{T}_h}, \phi_{\mathcal{T}_h})_{L^2}| \lesssim h^{2r+2}\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}, \\
|\xi_2| &\leq |\phi_h|_{s_h}|\hat{u}_h|_{s_h} \lesssim h^{r+2}\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}, \\
|\xi_3| &\leq |(\nabla_h(u - \mathcal{G}_h u), \nabla_h(\psi_{e_{\mathcal{T}_h}} - \mathcal{G}_h \psi_{e_{\mathcal{T}_h}}))_{L^2}| \\
&\qquad + |(\nabla_h(u - \mathcal{G}_h u), \nabla(\psi_{e_{\mathcal{T}_h}} - \mathcal{J}_h \hat{\phi}_h))_{L^2}| \lesssim h^{r+2}\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}, \\
|\xi_4| &\leq |(\Delta u - \Pi_{\mathcal{T}_h}^{k+1}\Delta u, \mathcal{J}_h \hat{\phi}_h - \psi_{e_{\mathcal{T}_h}})_{L^2}| \\
&\qquad + |(\Delta u - \Pi_{\mathcal{T}_h}^{k+1}\Delta u, \psi_{e_{\mathcal{T}_h}} - \phi_{\mathcal{T}_h})_{L^2}| \lesssim h^{r+2}\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}, \\
|\xi_5| &\lesssim \|\mathcal{J}_h \hat{e}_h - e_{\mathcal{T}_h}\|_{L^2}\|\phi_{\mathcal{T}_h}\|_{L^2} \lesssim h\|\nabla \mathcal{J}_h \hat{e}_h\|_{L^2}\|\phi_{\mathcal{T}_h}\|_{L^2} \lesssim h^{r+2}\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}, \\
|\xi_6| &\lesssim \|u - \Pi_{\mathcal{T}_h}^{k+1} u\|_{L^2}\|\phi_{\mathcal{T}_h}\|_{L^2} \lesssim h^{r+2}\|\psi_{e_{\mathcal{T}_h}}\|_{H^2}.
\end{aligned}
$$

Note that the estimate for ξ_1 uses arguments similar to those in (4.20) together with $(\phi_{\mathcal{T}_h}, u)_{L^2} = 0$, while the estimate for ξ_4 relies on the identity $(V + \kappa u^2 - \lambda)u = \Delta u$. Combining these estimates with the H^2-regularity bound $\|\psi_{e_{\mathcal{T}_h}}\|_{H^2} \lesssim \|e_{\mathcal{T}_h}\|_{L^2}$, we obtain for the first term on the right-hand side of (4.31) that

$$
|(\nabla \mathcal{J}_h \hat{e}_h, \nabla_h \mathcal{R}_h \hat{\phi}_h)_{L^2} + ((V + 3\kappa u^2 - \lambda)\mathcal{J}_h \hat{e}_h, \phi_{\mathcal{T}_h})_{L^2}| \lesssim h^{r+2}\|e_{\mathcal{T}_h}\|_{L^2}.
$$

For the second term on the right-hand side of (4.31), we obtain

$$
\begin{aligned}
&|(\nabla \mathcal{J}_h \hat{e}_h, \nabla \psi_{e_{\mathcal{T}_h}} - \nabla_h \mathcal{R}_h \hat{\phi}_h)_{L^2} + ((V + 3\kappa u^2 - \lambda)\mathcal{J}_h \hat{e}_h, \psi_{e_{\mathcal{T}_h}} - \phi_{\mathcal{T}_h})_{L^2}| \\
&\lesssim \|\nabla \mathcal{J}_h \hat{e}_h\|_{L^2}\|\nabla \psi_{e_{\mathcal{T}_h}} - \nabla_h \mathcal{R}_h \hat{\phi}_h\|_{L^2} + \|\mathcal{J}_h \hat{e}_h\|_{L^2}\|\psi_{e_{\mathcal{T}_h}} - \phi_{\mathcal{T}_h}\|_{L^2} \lesssim h^{r+2}\|e_{\mathcal{T}_h}\|_{L^2},
\end{aligned}
$$

where we applied Lemma A.4 and (4.29) to estimate the first term, and (4.30) together with the H^1-continuity of $\mathcal{J}_h$ for the second term.

We have now estimated both terms in the expression for Ξ_1 from (4.31). Combining these estimates yields the bound

$$
|\Xi_1| \lesssim h^{r+2}\|e_{\mathcal{T}_h}\|_{L^2},
$$

and the desired improved L^2-estimate, which is the first inequality in (4.23), follows directly by combining the estimates for Ξ_1–Ξ_3 and $\|u - \Pi_{\mathcal{T}_h}^{k+1} u\|_{L^2} \lesssim h^{r+2}$. Given the improved L^2-estimate, the refined eigenvalue approximation from (4.24) follows as

$$
|\lambda - \lambda_h| \leq 2|E - E_h| + \tfrac{\kappa}{2}|\|u\|_{L^4}^4 - \|u_{\mathcal{T}_h}\|_{L^4}^4| \lesssim h^{r+2}.
$$

To establish the refined L^2-estimate for the reconstructed approximation, we begin with the triangle inequality, which gives

$$\|\mathcal{R}_h \hat{u}_h - u\|_{L^2} \leq \|\mathcal{R}_h \hat{u}_h - \mathcal{R}_h \mathcal{I}_h u\|_{L^2} + \|\mathcal{G}_h u - u\|_{L^2}. \tag{4.32}$$

For estimating the first term on the right-hand side, we add and subtract the L^2-projection onto piecewise constants and apply the Poincaré inequality from Lemma A.1, along with Theorem 4.5 and the approximation properties of the Galerkin projection. This yields the estimate

$$\begin{aligned}\|\mathcal{R}_h \hat{u}_h - \mathcal{R}_h \mathcal{I}_h u\|_{L^2} &\lesssim \|h\nabla_h(\mathcal{R}_h \hat{u}_h - \mathcal{R}_h \mathcal{I}_h u)\|_{L^2} + \|\Pi^0_{\mathcal{T}_h}(\mathcal{R}_h \hat{u}_h - \mathcal{R}_h \mathcal{I}_h u)\|_{L^2} \\ &= \|h\nabla_h(\mathcal{R}_h \hat{u}_h - \mathcal{G}_h u)\|_{L^2} + \|\Pi^0_{\mathcal{T}_h}(u_{\mathcal{T}_h} - \Pi^{k+1}_{\mathcal{T}_h} u)\|_{L^2} \lesssim h^{r+2}.\end{aligned}$$

The second term on the right-hand side of (4.32) can be estimated in the same way, noting that the Galerkin projection preserves element averages by definition, and again using the Poincaré inequality from Lemma A.1. The refined L^2-estimate for the reconstruction, which is the second bound in (4.23), follows directly. □

The eigenvalue estimate in (4.24) appears suboptimal compared to the energy estimate in (4.17), noting that eigenvalue and energy approximations typically converge at the same rate. The following remark shows that, under suitable regularity assumptions, optimal convergence for the eigenvalue can be recovered.

Remark 4.7 (Optimal eigenvalue approximation). Assume that $u^3 \in H^m(\Omega)$ for some $0 \leq m \leq r$, and that the solution ψ_{u^3} to the dual problem (4.25) with right-hand side $w = u^3$ satisfies $\psi_{u^3} \in H^{m+2}(\Omega)$ with the estimate $\|\psi_{u^3}\|_{H^{m+2}} \lesssim \|u^3\|_{H^m}$. Then there holds the improved eigenvalue approximation result

$$|\lambda - \lambda_h| \lesssim h^{r+m+2}.$$

The proof of this result proceeds similarly to that of the improved L^2-error estimate in Theorem 4.6, now using dual problem (4.25) with the right-hand side $w = u^3$. This explains the regularity assumptions above. For brevity, the details are omitted here; we refer, for example, to [HY24], where the corresponding proof is carried out for a classical high-order conforming finite element method.

Thus far, we have conducted an error analysis of HHO approximation (2.4) to the Gross–Pitaevskii ground state. We now turn our attention to the analysis of its modified variant, defined in (3.2), which achieves guaranteed lower bounds for the ground state energy. Recall that only the lowest-order case $k = 0$ is of interest for the modified approximation, as the low-order quadrature in (3.2) prevents improved convergence rates for $k > 0$. Similar as for the classical HHO ground state approximation (2.4), also any discrete ground state of its modified variant (3.2) satisfies a discrete eigenvalue problem. It seeks an eigenpair $(\hat{u}^0_h, \lambda^0_h) \in \hat{U}_h \times \mathbb{R}$ with $\|u^0_{\mathcal{T}_h}\|_{L^2} = 1$ such that, for all $\hat{v}_h \in \hat{U}_h$, it holds that

$$a_h(\hat{u}^0_h, \hat{v}_h) + (V u^0_{\mathcal{T}_h}, v_{\mathcal{T}_h})_{L^2} + \kappa n_h(\hat{u}^0_h, \hat{v}_h) = \lambda^0_h (u^0_{\mathcal{T}_h}, v_{\mathcal{T}_h})_{L^2}, \tag{4.33}$$

where the nonlinearity is encoded in the form n_h, defined for any $\hat{v}_h, \hat{\varphi}_h \in \hat{U}_h$, as

$$n_h(\hat{v}_h, \hat{\varphi}_h) := \tfrac{1}{2}\big((\Pi^0_{\mathcal{T}_h} v_{\mathcal{T}_h})^2 v_{\mathcal{T}_h}, \varphi_{\mathcal{T}_h}\big)_{L^2} + \tfrac{1}{2}\big((v_{\mathcal{T}_h})^2 \Pi^0_{\mathcal{T}_h} v_{\mathcal{T}_h}, \Pi^0_{\mathcal{T}_h} \varphi_{\mathcal{T}_h}\big)_{L^2}.$$

The following theorem summarises the convergence results for the modified HHO approximation. As the proof follows that of the standard HHO method, we keep the presentation short and directly state the final result.

Theorem 4.8 (A priori error estimate)**.** *Assume that $V \in H^1(\mathcal{T}_h)$. Then, the approximation of the modified HHO method satisfies the following estimates:*

$$\|\nabla_h(\mathcal{R}_h \hat{u}^0_h - u)\|_{L^2} + |\hat{u}^0_h|_{s_h} + |\hat{u}^0_h - \mathcal{I}_h u|_{s_h} \lesssim h.$$

Moreover, the ground state approximation satisfies the L^2-error bounds

$$\|u^0_{\mathcal{T}_h} - u\|_{L^2} + \|\mathcal{R}_h \hat{u}^0_h - u\|_{L^2} \lesssim h^2,$$

and the energy and eigenvalue approximations satisfy

$$|E - E^0_h| \lesssim h^2, \quad |\lambda - \lambda^0_h| \lesssim h^2.$$

Proof. As before, one first needs to establish the plain convergence of the modified HHO method. The proof is very similar to that of Theorem 4.2 for the classical HHO method and is therefore omitted. As a direct consequence, we obtain the uniform boundedness of the modified discrete energies E^0_h, as well as the uniform boundedness of $\|u^0_{\mathcal{T}_h}\|_{L^6}$ via the discrete Sobolev embedding from Lemma A.3. Furthermore, Lemma A.5 ensures the uniform boundedness of $\|u^0_{\mathcal{T}_h}\|_{L^\infty}$ and $\|\mathcal{J}_h \hat{u}^0_h\|_{L^\infty}$. Next, repeating the arguments from Lemmas 4.3 and 4.4, Theorems 4.5 and 4.6, and using Lemma A.7 to bound the quadrature errors together with Proposition A.6, we also obtain the desired convergence properties of the modified HHO approximation. □

5. Numerical experiments

This section presents numerical experiments that validate the theory and demonstrate the method's practical effectiveness. To solve the finite-dimensional constrained minimisation problems (2.4) and (3.2), we employ solvers specifically tailored to their structure. Of the available approaches (see [HJ25] for an overview), we employ an adaptation of the (fully discrete) energy-adaptive Sobolev gradient flow from [HP20], together with an adaptive choice of step sizes (see Remark 4.3 of that paper). The initial iterate is constructed by setting all interior degrees of freedom to one and all boundary degrees of freedom to zero. The resulting function is normalised with respect to the discrete L^2-norm to obtain a suitable initial guess. The iteration is terminated if the relative L^2-residual of the current iterate and the relative energy difference between two consecutive iterates falls below 10^{-12}. The maximal number of iterations is 10^3. Details on the implementation can be found in the code available at `https://github.com/moimmahauck/GPE_HHO_code`, which is based on an implementation of the HHO method used for [Tra24]. The latter, in turn, is based on the basic finite element implementation detailed in [ACF99].

All of our numerical experiments consider the domain $\Omega = (-8, 8)^2$ and a hierarchy of Friedrichs–Keller triangulations constructed by uniform red refinement of an initial triangulation of the domain consisting of two elements. We exclude the coarsest meshes from this hierarchy since they do not resolve the considered potentials and therefore do not yield meaningful approximations. To simplify the notation, we denote the side length of the squares formed by joining opposing triangles by h. Since analytical solutions are typically not available, errors are computed with respect to the Q^{k+1}-finite element approximation on the uniform Cartesian grid obtained by twice uniform red refinement of the finest mesh in the hierarchy and joining opposing triangles. With a slight abuse of notation, we denote its energy, eigenvalue, and ground state approximations by E, λ, and u, respectively.

5.1. Guaranteed lower energy bounds.

To investigate the guaranteed lower energy bounds provided by the modified HHO method from (3.2), we present three numerical experiments. The *first experiment* considers the harmonic potential $V_1(x) := \frac{1}{2}|x|^2$, with the particle interaction parameter set to $\kappa = 1000$. In the *second experiment*, we use the so-called *lattice potential*, defined as

$$V_2(x) := \tfrac{1}{2}|x|^2 + 15\left(1 + \sin\left(\tfrac{\pi x_1}{2}\right)\sin\left(\tfrac{\pi x_2}{2}\right)\right),$$

again with $\kappa = 1000$. The *third experiment* involves a disorder potential, denoted by V_3, which is piecewise constant on a Cartesian grid with mesh size $h = 2^0$. The

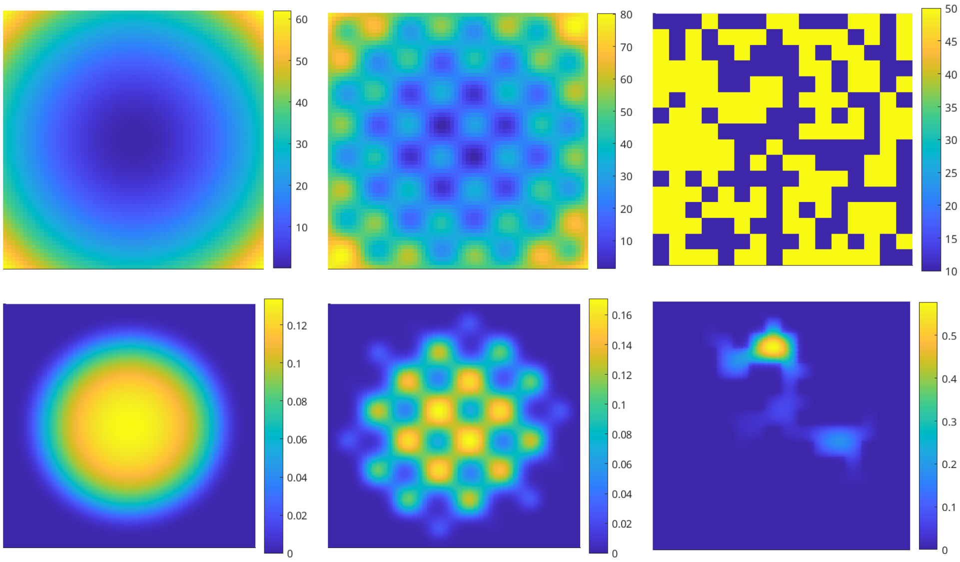

FIGURE 5.1. First row: Potentials V_1, V_2, and V_3 (from left to right). Second row: corresponding ground state approximations.

values on each grid element are assigned randomly as independent realisations of coin-toss variables taking values in $\{10, 50\}$. The particle interaction parameter is set to $\kappa = 1$. Illustrations of the potentials and corresponding ground state approximations are provided in Figure 5.1. Note that for the disorder potential, a phenomenon known as Anderson localisation occurs (see, e.g., [AHP20, AHP22]), which leads to an exponential localisation of the ground state.

We consider the mesh hierarchy $\{\mathcal{T}_h : h = 2^{-3}, \dots, 2^{-7}\}$. To satisfy the assumption of a piecewise constant potential required in Theorem 3.1, the potentials V_1 and V_2 are projected onto the space of piecewise constant functions defined on a uniform Cartesian grid with mesh size $h = 2^{-2}$. The potentials on all finer meshes are obtained via prolongation. The computations are carried out using the modified HHO method introduced in (3.2), where the stabilisation parameter σ is determined by rearranging (3.5) for σ and estimating E_h^0 from above using the reference energy E, which is computed via the conforming $\mathcal{Q}^1$-finite element method (as outlined above). For the considered mesh sizes, the resulting stabilisation parameter is of order one, and it satisfies the condition in (3.5) by construction.

The first row of Figure 5.2 confirms that the energy approximation E_h^0 indeed provides guaranteed lower energy bounds, as theoretically predicted by Theorem 3.1. For comparison, we also show the post-processed energy approximations obtained using the lowest-order Raviart–Thomas discretisation from [GHLP25], which also yields guaranteed lower energy bounds. The second row of Figure 5.2 displays the energy approximation errors for the modified HHO method and the post-processed Raviart–Thomas method. Notably, for the potentials V_1 and V_2, the modified HHO method yields significantly more accurate lower bounds (by approximately two orders of magnitude for V_1 and one and a half orders for V_2) compared to the Raviart–Thomas method. The discrepancy arises from the post-processing step in the Raviart–Thomas method, which dominates the error in case of the smooth potentials V_1 and V_2, where the discretisation error is comparatively small. For the rough potential V_3, the lower energy bounds provided by the modified HHO method are still more accurate than that of the post-processed Raviart–Thomas method, though the improvement is less pronounced (about a factor of three).

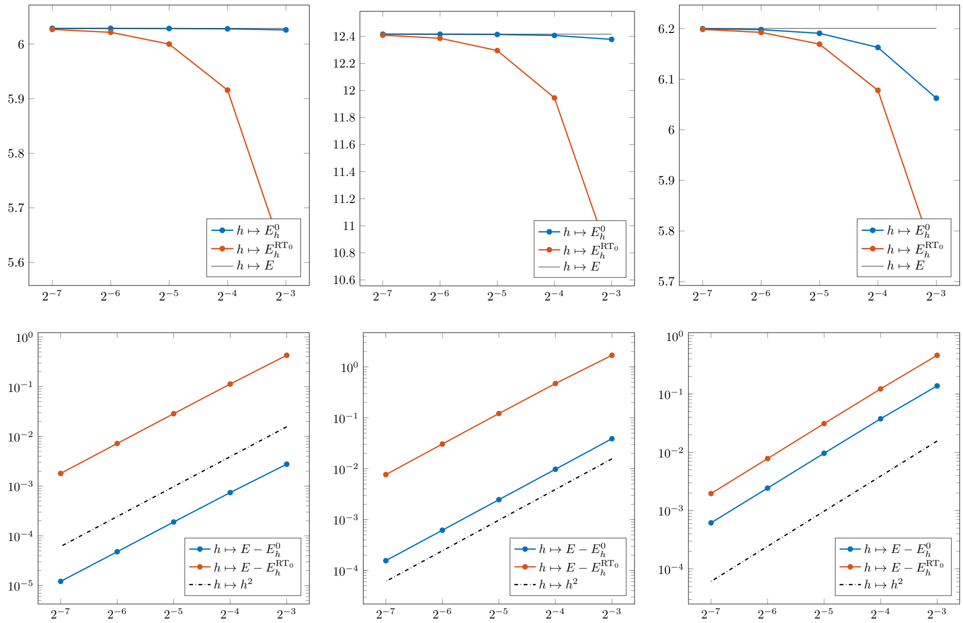

FIGURE 5.2. First row: energy approximations E_h^0 of the modified HHO method and $E_h^{\mathrm{RT}_0}$ of the post-processed Raviart–Thomas method (see [GHLP25]) for the potentials V_1, V_2, and V_3 (from left to right). Second row: corresponding approximation errors.

5.2. **Optimal order convergence.** In the following, we investigate the convergence properties of the HHO method introduced in (2.4) and its modified version from (3.2). For the corresponding numerical experiments, we consider the harmonic potential V_1 and set the particle interaction parameter to $\kappa = 1000$. The potential is integrated exactly using a quadrature rule of sufficiently high order.

To demonstrate the convergence of the HHO method introduced in (2.4), we employ the mesh hierarchy $\{\mathcal{T}_h : h = 2^0, \dots, 2^{-4}\}$. In Figure 5.3 one observes that the HHO method exhibits optimal convergence rates, in agreement with the theoretical predictions of Theorems 4.5 and 4.6. Note that, both $\|u - u_{\mathcal{T}_h}\|_{L^2}$ and $\|u - \mathcal{R}_h \hat{u}_h\|_{L^2}$ converge at the expected rate of $\mathcal{O}(h^{k+2})$; however, for polynomial degrees $k > 0$, the latter error is consistently smaller by approximately one order of magnitude. In the lower-left plot of Figure 5.3, one observes that the eigenvalue approximation for the HHO method with polynomial degree $k = 2$ stagnates at an error level of approximately 10^{-8}. This behavior is likely due to numerical effects such as finite machine precision and the stopping criteria of the nonlinear solver.

For the modified HHO method, we consider the mesh hierarchy $\{\mathcal{T}_h : h = 2^0, \dots, 2^{-6}\}$. After an initial plateau in the error, which is due to the nonlinear solver for (3.2) not converging within the maximum number of iterations, the expected convergence rate predicted by Theorem 4.8 is clearly observed.

6. Conclusion

In conclusion, we have demonstrated the effective application of a hybrid high-order (HHO) discretisation to the Gross–Pitaevskii eigenvalue problem. We have proved the optimal-order convergence both for the classical HHO ground state approximation and for a modified lowest-order variant that provides guaranteed lower bounds on the ground state energy. Notably, these bounds are obtained without

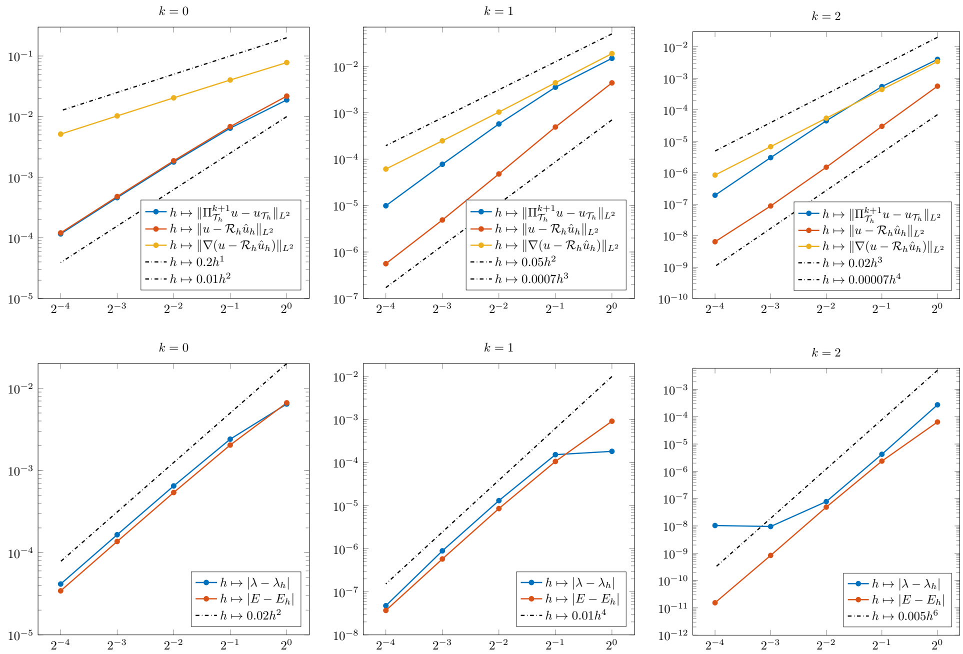

FIGURE 5.3. First row: convergence plots of the (reconstructed) ground state approximations of the HHO method for polynomial degrees $k = 1, 2, 3$ (from left to right). Second row: convergence plots of the corresponding eigenvalue and energy approximations.

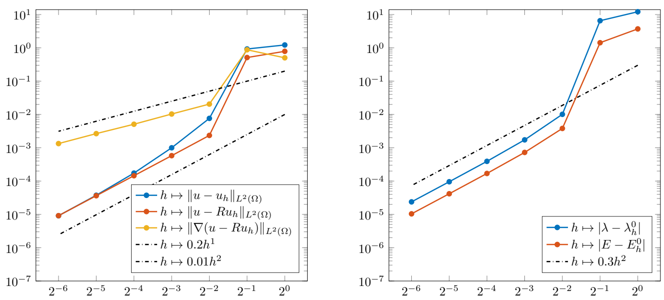

FIGURE 5.4. Left: convergence plot of the ground state approximation of the modified HHO method. Right: convergence plot of the corresponding eigenvalue and energy approximations (right).

any post-processing. Numerical experiments confirm that, particularly for smooth problems, the proposed method produces significantly more accurate guaranteed lower energy bounds than the post-processing-based approach [GHLP25].

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Appendix A. Collection of frequently used bounds

The first two results are a Poincaré inequality and a trace inequality, both stated with explicit constants.

Lemma A.1 (Poincare inequality)**.** *For all $T \in \mathcal{T}_h$ and any $v \in H^1(T)$ with $\int_T v\,\mathrm{d}x = 0$, it holds that*

$$\|v\|_{L^2(T)} \le \pi^{-1} h_T \|\nabla v\|_{L^2(T)}$$

with $\pi > 0$ denoting the circle constant.

Proof. The proof can be found, for example, in [Beb03]. □

Lemma A.2 (Trace inequality)**.** *For all $T \in \mathcal{T}_h$ and any $v \in H^1(T)$ satisfying $\int_T v\,\mathrm{d}x = 0$, it holds that*

$$\sum_{F \in \mathcal{F}_{\partial T}} \ell_{T,F}^{-1} \|u\|_{L^2(F)}^2 \le C_{\mathrm{tr}} \|\nabla u\|_{L^2(T)}^2$$

with the constant $C_{\mathrm{tr}} = 1/\pi^2 + 2/(d\pi) > 0$.

Proof. The result and its corresponding proof can be found in [Tra24, Lem. 3.1], which, in turn, is based on [Gal23, Lem. 7.2]. □

Next, we present several results relevant to the analysis of the HHO method.

Lemma A.3 (Discrete Sobolev embeddings)**.** *Let $d \in \{2, 3\}$ and q satisfy $1 \le q < \infty$ if $d = 2$, and $1 \le q \le 6$ if $d = 3$. Then, for all $\hat{v}_h = (v_{\mathcal{T}_h}, v_{\mathcal{F}_h}) \in \hat{U}_h$, it holds that*

$$\|v_{\mathcal{T}_h}\|_{L^q} \lesssim \|\hat{v}_h\|_{a_h}$$

with hidden constant depending only on the domain, mesh regularity, q, k, and σ.

Proof. The proof of this result can be deduced by combining [DPD17, Prop. 5.4] and [DPD20, Lem. 2.18]. □

Lemma A.4 (Moment-preserving smoothing operator)**.** *There exists a linear operator $\mathcal{J}_h \colon \hat{U}_h \to H_0^1(\Omega)$ satisfying, for all $\hat{v}_h \in \hat{U}_h$, that*

$$\mathcal{I}_h \circ \mathcal{J}_h \hat{v}_h = \hat{v}_h,$$

which implies the following orthogonality relations:

$$v_{\mathcal{T}_h} - \mathcal{J}_h \hat{v}_h \perp_{L^2} \mathcal{P}^{k+1}(\mathcal{T}_h), \quad \nabla_h(\mathcal{J}_h \hat{v}_h - \mathcal{R}_h \hat{v}_h) \perp_{L^2} \nabla_h \mathcal{P}^{k+1}(\mathcal{T}_h).$$

Moreover, the operator satisfies, for all $\hat{v}_h \in \hat{U}_h$, the stability estimate

$$\|\mathcal{J}_h \hat{v}_h\|_{H^1} \lesssim \|\hat{v}_h\|_{a_h},$$

and, for any $v \in H^2(\Omega) \cap H_0^1(\Omega)$, the following approximation properties hold:

$$\|\nabla(\mathcal{J}_h \mathcal{I}_h v - v)\|_{L^2} \lesssim h\|v\|_{H^2}, \quad \|\mathcal{J}_h \mathcal{I}_h v - v\|_{L^2} \lesssim h^2 \|v\|_{H^2},$$

where hidden constants depend only on the domain, mesh regularity, k, and σ.

Proof. For the construction of such an operator and the corresponding analysis, we refer, for example, to [EZ20, Sec. 4.3]. The proof of the stability and approximation properties uses similar arguments as [LT25, Lem. 3.5]. □

Lemma A.5 (Discrete L^∞-bound)**.** *Assume that $V \in H^1(\mathcal{T}_h)$. Then, for any discrete ground state $\hat{u}_h = (u_{\mathcal{T}_h}, u_{\mathcal{F}_h})$ of (2.4), both $\|\mathcal{J}_h \hat{u}_h\|_{L^\infty}$ and $\|u_{\mathcal{T}_h}\|_{L^\infty}$ are uniformly bounded. The same holds for the modified HHO approximation $\hat{u}_h^0 = (u_{\mathcal{T}_h}^0, u_{\mathcal{F}_h}^0)$ of (3.2) and its smoothed version $\mathcal{J}_h \hat{u}_h^0$.*

Proof. We proceed as in the proof of Theorem 4.2, observing that $\hat{u}_h$ can be interpreted as the HHO approximation of the solution $u_h^c \in H^2(\Omega) \cap H_0^1(\Omega)$ to the auxiliary Poisson problem (4.3). Recall that the H^2-norm of u_h^c is uniformly bounded. The improved L^2-error estimate for the HHO method, as established for example in [DPD20, Thm. 2.32 & 2.33], then implies that

$$\|\mathcal{R}_h \hat{u}_h - u_h^c\|_{L^2} + \|\Pi_{\mathcal{T}_h}^{k+1} u_h^c - u_{\mathcal{T}_h}\|_{L^2} \lesssim h^2.$$

Using a comparison between the discrete L^2- and L^∞-norms, the stability of the L^2-projection, and the uniform L^∞-bound for u_h^c, we obtain for any $T \in \mathcal{T}_h$ that

$$\begin{aligned}
\|u_{\mathcal{T}_h}\|_{L^\infty(T)} &\leq \|\Pi_{\mathcal{T}_h}^{k+1} u_h^c - u_{\mathcal{T}_h}\|_{L^\infty(T)} + \|\Pi_{\mathcal{T}_h}^{k+1} u_h^c\|_{L^\infty(T)} \\
&\lesssim h_T^{-d/2} \|\Pi_{\mathcal{T}_h}^{k+1} u_h^c - u_{\mathcal{T}_h}\|_{L^2(T)} + h_T^{-d/2} \|u_h^c\|_{L^2(T)} \\
&\lesssim h_T^{(4-d)/2} + \|u_h^c\|_{L^\infty(T)} \lesssim 1.
\end{aligned}$$

Similarly arguments also show that $\mathcal{R}_h \hat{u}_h$ is uniformly L^∞-bounded.

Next, we show that $\mathcal{J}_h \hat{u}_h$ is uniformly L^∞-bounded. Using again the comparison result between discrete norms, we obtain for any $T \in \mathcal{T}_h$ that

$$\begin{aligned}
\|\mathcal{J}_h \hat{u}_h\|_{L^\infty(T)} &\lesssim h_T^{-d/2} \|\mathcal{J}_h \hat{u}_h\|_{L^2(T)} \\
&\lesssim h_T^{-d/2} \sum_{T' \cap T \neq \emptyset} \Big\{ \|\mathcal{R}_h \hat{u}_h\|_{L^2(T')} + \|\mathcal{R}_h \hat{u}_h - u_{\mathcal{T}_h}\|_{L^2(T')} \\
&\qquad + \sum_{F \in \mathcal{F}_{\partial T'}} h_F^{1/2} \|\Pi_F^k (\mathcal{R}_h \hat{u}_h - u_{\mathcal{F}_h})\|_{L^2(F)} \Big\} \\
&\lesssim \|\mathcal{R}_h \hat{u}_h\|_{L^\infty} + \|\mathcal{R}_h \hat{u}_h - u_{\mathcal{T}_h}\|_{L^\infty} + h^{-(d-2)/2} |\hat{u}_h|_{s_h} \lesssim 1,
\end{aligned}$$

where the second inequality follows from the specific construction of $\mathcal{J}_h$ in [EZ20, Sec. 4.3], and arguments similar to those in [LT25, Lem. 3.5]. To derive the last inequality, we use that $|\hat{u}_h|_{s_h} \lesssim h \|u_h^c\|_{H^2}$ (see Theorem 4.5 or [DPD20, Thm. 2.28]). This leads the uniform L^∞-bound for $\mathcal{J}_h \hat{u}_h$. The corresponding proof for the modified HHO approximation $\hat{u}_h^0$ is analogous and is therefore omitted for brevity. □

Proposition A.6. *For any $v \in H^2(\Omega) \cap H_0^1(\Omega)$, it holds that*

$$\|\mathcal{J}_h \mathcal{I}_h v\|_{L^\infty} \lesssim \|\mathcal{R}_h \mathcal{I}_h v\|_{L^\infty} + \|\mathcal{R}_h \mathcal{I}_h v - \Pi_{\mathcal{T}_h}^{k+1} v\|_{L^\infty} + h^{-(d-2)/2} |\mathcal{I}_h v|_{s_h} \lesssim \|v\|_{H^2}.$$

Lemma A.7 (Quadrature error)**.** *For any $\hat{v}_h = (v_{\mathcal{T}_h}, v_{\mathcal{F}_h})$, $\hat{w}_h = (w_{\mathcal{T}_h}, w_{\mathcal{F}_h}) \in \hat{U}_h$, we have the following two estimates:*

$$\tag{A.1} \begin{aligned}
&|((\Pi_{\mathcal{T}_h}^0 v_{\mathcal{T}_h})^2 - v_{\mathcal{T}_h}^2, v_{\mathcal{T}_h} w_{\mathcal{T}_h})_{L^2}| \\
&\lesssim h^2 \|v_{\mathcal{T}_h}\|_{L^\infty} \|\nabla \mathcal{J}_h \hat{v}_h\|_{L^2} \big(\|v_{\mathcal{T}_h}\|_{L^\infty} \|\nabla \mathcal{J}_h \hat{w}_h\|_{L^2} + \|\nabla \mathcal{J}_h \hat{v}_h\|_{L^2} \|\mathcal{J}_h \hat{w}_h\|_{L^\infty} \\
&\qquad + \|\mathcal{J}_h \hat{v}_h\|_{L^\infty} \|\nabla \mathcal{J}_h \hat{w}_h\|_{L^2} + \|w_{\mathcal{T}_h}\|_{L^\infty} \|\nabla \mathcal{J}_h \hat{v}_h\|_{L^2} \big),
\end{aligned}$$

$$\tag{A.2} \begin{aligned}
&|(v_{\mathcal{T}_h}^2, v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \Pi_{\mathcal{T}_h}^0 v_{\mathcal{T}_h} \Pi_{\mathcal{T}_h}^0 w_{\mathcal{T}_h})_{L^2}| \\
&\lesssim h^2 \big(\|v_{\mathcal{T}_h}\|_{L^\infty} \|\nabla \mathcal{J}_h \hat{v}_h\|_{L^2} + \|\mathcal{J}_h \hat{v}_h\|_{L^\infty} \|\nabla \mathcal{J}_h \hat{v}_h\|_{L^2} \big) \\
&\qquad \times \big(\|v_{\mathcal{T}_h}\|_{L^\infty} \|\nabla \mathcal{J}_h \hat{w}_h\|_{L^2} + \|w_{\mathcal{T}_h}\|_{L^\infty} \|\nabla \mathcal{J}_h \hat{v}_h\|_{L^2} \big),
\end{aligned}$$

where hidden constants depend only on the domain, mesh regularity, k, and σ.

Proof. We begin the proof by establishing three auxiliary estimates that will be used later. The first one, which holds for any $\hat{v}_h = (v_{\mathcal{T}_h}, v_{\mathcal{F}_h}) \in \hat{U}_h$, reads

$$\tag{A.3} \|v_{\mathcal{T}_h} - \Pi_{\mathcal{T}_h}^0 v_{\mathcal{T}_h}\|_{L^2} \leq \|v_{\mathcal{T}_h} - \mathcal{J}_h \hat{v}_h\|_{L^2} + \|\mathcal{J}_h \hat{v}_h - \Pi_{\mathcal{T}_h}^0 v_{\mathcal{T}_h}\|_{L^2} \lesssim h \|\nabla \mathcal{J}_h \hat{v}_h\|_{L^2}.$$

This follows from $\Pi^{k+1}_{\mathcal{T}_h}\mathcal{J}_h\hat{v}_h = v_{\mathcal{T}_h}$ and the approximation properties of the L^2-projection. To derive the second estimate, we apply the triangle inequality along with the first estimate, which gives, for any $\hat{v}_h, \hat{w}_h \in \hat{U}_h$, that

(A.4)
$$\begin{aligned}\|v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \mathcal{J}_h\hat{v}_h\mathcal{J}_h\hat{w}_h\|_{L^2} &\leq \|v_{\mathcal{T}_h} w_{\mathcal{T}_h} - v_{\mathcal{T}_h}\mathcal{J}_h\hat{w}_h\|_{L^2} + \|v_{\mathcal{T}_h}\mathcal{J}_h\hat{w}_h - \mathcal{J}_h\hat{v}_h\mathcal{J}_h\hat{w}_h\|_{L^2}\\ &\lesssim h\|v_{\mathcal{T}_h}\|_{L^\infty}\|\nabla\mathcal{J}_h\hat{w}_h\|_{L^2} + h\|\mathcal{J}_h\hat{w}_h\|_{L^\infty}\|\nabla\mathcal{J}_h\hat{v}_h\|_{L^2}.\end{aligned}$$

To prove the third estimate, we use the triangle inequality, the approximation properties of the L^2-projection, and the product rule, which yields that

(A.5)
$$\begin{aligned}&\|v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \Pi^0_{\mathcal{T}_h}(v_{\mathcal{T}_h} w_{\mathcal{T}_h})\|_{L^2}\\ &\quad\leq \|v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \mathcal{J}_h\hat{v}_h\mathcal{J}_h\hat{w}_h\|_{L^2} + \|\mathcal{J}_h\hat{v}_h\mathcal{J}_h\hat{w}_h - \Pi^0_{\mathcal{T}_h}(\mathcal{J}_h\hat{v}_h\mathcal{J}_h\hat{w}_h)\|_{L^2}\\ &\qquad + \|\Pi^0_{\mathcal{T}_h}(v_{\mathcal{T}_h} w_{\mathcal{T}_h}) - \Pi^0_{\mathcal{T}_h}(\mathcal{J}_h\hat{v}_h\mathcal{J}_h\hat{w}_h)\|_{L^2}\\ &\quad\lesssim h\big(\|v_{\mathcal{T}_h}\|_{L^\infty}\|\nabla\mathcal{J}_h\hat{w}_h\|_{L^2} + \|\nabla\mathcal{J}_h\hat{v}_h\|_{L^2}\|\mathcal{J}_h\hat{w}_h\|_{L^\infty} + \|\mathcal{J}_h\hat{v}_h\|_{L^\infty}\|\nabla\mathcal{J}_h\hat{w}_h\|_{L^2}\big).\end{aligned}$$

We now have the tools to prove (A.1). Applying the triangle inequality yields

$$\begin{aligned}|((\Pi^0_{\mathcal{T}_h}v_{\mathcal{T}_h})^2 - v^2_{\mathcal{T}_h}, v_{\mathcal{T}_h} w_{\mathcal{T}_h})_{L^2}| &\leq \underbrace{|((\Pi^0_{\mathcal{T}_h}v_{\mathcal{T}_h})^2 - v^2_{\mathcal{T}_h}, \Pi^0_{\mathcal{T}_h}(v_{\mathcal{T}_h} w_{\mathcal{T}_h}))_{L^2}|}_{=:\Xi_1}\\ &\quad + \underbrace{|((\Pi^0_{\mathcal{T}_h}v_{\mathcal{T}_h})^2 - v^2_{\mathcal{T}_h}, v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \Pi^0_{\mathcal{T}_h}(v_{\mathcal{T}_h} w_{\mathcal{T}_h}))_{L^2}|}_{=:\Xi_2},\end{aligned}$$

where the term Ξ_1 can be estimated as

(A.6)
$$\Xi_1 \leq \sum_{T\in\mathcal{T}_h}|\Pi^0_T(v_T w_T)|\int_T (v_T - \Pi^0_T v_T)^2\mathrm{d}x \lesssim h^2\|v_{\mathcal{T}_h}\|_{L^\infty}\|w_{\mathcal{T}_h}\|_{L^\infty}\|\nabla\mathcal{J}_h\hat{v}_h\|^2_{L^2}.$$

Here, the first inequality follows from elementary algebraic manipulations, using $\Pi^0_T v = |T|^{-1}\int_T v\,\mathrm{d}x$, while the second follows from $\|\Pi^0_T v\|_{L^\infty(T)} \leq \|v\|_{L^\infty(T)}$ and (A.3). The term Ξ_2 can be estimated as

$$\Xi_2 \lesssim h\|v_{\mathcal{T}_h}\|_{L^\infty}\|\nabla\mathcal{J}_h\hat{v}_h\|_{L^2}\|v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \Pi^0_{\mathcal{T}_h}(v_{\mathcal{T}_h} w_{\mathcal{T}_h})\|_{L^2},$$

where we again use the L^∞-bound of Π^0_T and (A.3). Applying (A.5) to estimate the last term on the right-hand side yields the desired bound for Ξ_2. Combining the previous estimates then establishes (A.1).

Next, we prove estimate (A.2). Applying the triangle inequality, we obtain that

$$\begin{aligned}|(v^2_{\mathcal{T}_h}, v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \Pi^0_{\mathcal{T}_h}v_{\mathcal{T}_h}\Pi^0_{\mathcal{T}_h}w_{\mathcal{T}_h})_{L^2}| &\leq \underbrace{|(\Pi^0_{\mathcal{T}_h}(v^2_{\mathcal{T}_h}), v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \Pi^0_{\mathcal{T}_h}v_{\mathcal{T}_h}\Pi^0_{\mathcal{T}_h}w_{\mathcal{T}_h})_{L^2}|}_{=:\xi_1}\\ &\quad + \underbrace{|(v^2_{\mathcal{T}_h} - \Pi^0_{\mathcal{T}_h}(v^2_{\mathcal{T}_h}), v_{\mathcal{T}_h} w_{\mathcal{T}_h} - \Pi^0_{\mathcal{T}_h}v_{\mathcal{T}_h}\Pi^0_{\mathcal{T}_h}w_{\mathcal{T}_h})_{L^2}|}_{=:\xi_2}.\end{aligned}$$

To estimate the term Ξ_1, we apply algebraic manipulations similar to those in the proof of (A.6), as well as the L^∞-bound of Π^0_T and (A.3), which gives

$$\begin{aligned}\xi_1 &\leq \sum_{T\in\mathcal{T}_h}|\Pi^0_T(v^2_T)||\int_T (v_T - \Pi^0_T v_T)(w_T - \Pi^0_T w_T)\mathrm{d}x|\\ &\lesssim h^2\|v_{\mathcal{T}_h}\|^2_{L^\infty}\|\nabla\mathcal{J}_h\hat{v}_h\|_{L^2}\|\nabla\mathcal{J}_h\hat{w}_h\|_{L^2}.\end{aligned}$$

The term ξ_2 can be estimated by applying (A.5) with $\hat{v}_h = \hat{w}_h$, proceeding similarly to the proof of (A.4). Combining these estimates yields (A.2). □

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* Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, Englerstr. 2, 76131 Karlsruhe, Germany
Email address: moritz.hauck@kit.edu

† School for Mathematics, University of Edinburgh, Mayfield Road, James Clerk Maxwell Building, EH9 3FD Edinburgh
Email address: yizhou.liang@ed.ac.uk