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TWO-LEVEL DISCRETIZATION TECHNIQUES FOR GROUND STATE COMPUTATIONS OF BOSE-EINSTEIN CONDENSATES[*]

PATRICK HENNING[†], AXEL MÅLQVIST[‡], AND DANIEL PETERSEIM[§]

Abstract. This work presents a new methodology for computing ground states of Bose–Einstein condensates based on finite element discretizations on two different scales of numerical resolution. In a preprocessing step, a low-dimensional (coarse) generalized finite element space is constructed. It is based on a local orthogonal decomposition of the solution space and exhibits high approximation properties. The nonlinear eigenvalue problem that characterizes the ground state is solved by some suitable iterative solver exclusively in this low-dimensional space, without significant loss of accuracy when compared with the solution of the full fine scale problem. The preprocessing step is independent of the types and numbers of bosons. A postprocessing step further improves the accuracy of the method. We present rigorous a priori error estimates that predict convergence rates H^3 for the ground state eigenfunction and H^4 for the corresponding eigenvalue without pre-asymptotic effects; H being the coarse scale discretization parameter. Numerical experiments indicate that these high rates may still be pessimistic.

Key words. eigenvalue, finite element, Gross–Pitaevskii equation, numerical upscaling, two-grid method, multiscale method

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

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1. Introduction. Bose–Einstein condensates (BEC) are formed when a dilute gas of trapped bosons (of the same species) is cooled down to ultra-low temperatures close to absolute zero [10, 19, 22, 38]. In this case, nearly all bosons are in the same quantum mechanical state, which means that they loose their identity and become indistinguishable from each other. The BEC therefore behaves like one "super particle" where the quantum state can be described by a single collective wave function Ψ. The dynamics of a BEC can be modeled by the time-dependent Gross–Pitaevskii equation (GPE) [26, 31, 37], which is a nonlinear Schrödinger equation given by

$$(1.1) \qquad i\hbar\,\partial_t\Psi = -\frac{\hbar^2}{2m}\Delta\Psi + V_e\Psi + \frac{4\pi\hbar^2 aN}{m}|\Psi|^2\Psi.$$

Here, m denotes the atomic mass of a single boson, N is the number of bosons (typically in the span between 10^3 and 10^7), $\hbar$ is the reduced Plank's constant, and V_e is an external trapping potential that confines the system. The nonlinear term in the equation describes the effective two-body interaction between the particles. If the scattering length a is positive, the interaction is repulsive; if it is negative the interaction is attractive. For $a = 0$ there is no interaction and (1.1) becomes the

corresponding eigenvalue $\lambda := 2E(u) + 2^{-1}\beta\|u\|^4_{L^4(\Omega)}$ of the GPE is real, positive, and simple. Observe that the eigenpair (u, λ) satisfies

$$\int_\Omega A\nabla u \cdot \nabla\phi\, dx + \int_\Omega bu\phi\, dx + \int_\Omega \beta|u|^2 u\phi\, dx = \lambda \int_\Omega u\phi\, dx$$

for all $\phi \in H_0^1(\Omega)$. Moreover, λ is the smallest among all possible eigenvalues and satisfies the a priori bound $\lambda < 4E(u)$.

3. Discretization. This section recalls classical finite element discretizations and presents novel two-grid approaches for the numerical solution of Problem 2.1. The existence of a minimizer of the functional E in discrete spaces is easily seen. However, uniqueness does not hold in general. We note that unlike as claimed in [44] the uniqueness proof given in [31] does not generalize to arbitrary subspaces of the original solution space.

Remark 3.1 (existence of discrete solutions [13]). Let W denote a finite dimensional, nonempty subspace of $H_0^1(\Omega)$; then there exists a minimizer $u_W \in W$ with $\|u_W\|_{L^2(\Omega)} = 1$, $(u_W, 1)_{L^2(\Omega)} \geq 0$, and

$$E(u_W) = \inf_{\substack{w \in W \\ \|w\|_{L^2(\Omega)}=1}} E(w).$$

If $(W_i)_{i\in\mathbb{N}}$ represents a dense family of such subspaces, then any sequence of corresponding minimizers $(u_i)_{i\in\mathbb{N}}$ with $(u_i, 1)_{L^2(\Omega)} \geq 0$ converges to the unique solution u of Problem 2.1.

3.1. Standard finite elements. We consider two regular simplicial meshes $\mathcal{T}_H$ and $\mathcal{T}_h$ of Ω. The finer mesh $\mathcal{T}_h$ is obtained from the coarse mesh $\mathcal{T}_H$ by regular mesh refinement. The discretization parameters $h \leq H$ represent the mesh size, i.e., $h_T := \operatorname{diam}(T)$ (resp., $H_T := \operatorname{diam}(T)$) for $T \in \mathcal{T}_h$ (resp., $\mathcal{T}_H$) and $h := \max_{T\in\mathcal{T}_h}\{h_T\}$ (resp., $H := \max_{T\in\mathcal{T}_H}\{H_T\}$). For $\mathcal{T} = \mathcal{T}_H, \mathcal{T}_h$, let

$$P_1(\mathcal{T}) = \{v \in L^2(\Omega) \mid \text{for all } T \in \mathcal{T}, v|_T \text{ is a polynomial of total degree} \leq 1\}$$

denote the set of $\mathcal{T}$-piecewise affine functions. Classical $H_0^1(\Omega)$-conforming finite element spaces are then given by

$$V_h := P_1(\mathcal{T}_h) \cap H_0^1(\Omega) \quad \text{and} \quad V_H := P_1(\mathcal{T}_H) \cap H_0^1(\Omega) \subset V_h.$$

Note that on the fine discretization scale, a different choice of polynomial degree, e.g., piecewise quadratic functions, is possible. This would be a better choice for smooth data that allows for a regular ground state. Our method and its analysis essentially require the inclusion $H_0^1(\Omega) \supset V_h \supset V_H$. The discrete problem on the fine grid $\mathcal{T}_h$ reads as follows.

Problem 3.2 (reference finite element discretization on the fine mesh). Find $u_h \in V_h$ with $(u_h, 1)_{L^2(\Omega)} \geq 0$, $\|u_h\|_{L^2(\Omega)} = 1$ and

$$(3.1) \qquad\qquad E(u_h) = \inf_{\substack{v_h \in V_h \\ \|v_h\|_{L^2(\Omega)}=1}} E(v_h).$$

The corresponding eigenvalue is given by $\lambda_h := 2E(u_h) + 2^{-1}\beta\|u_h\|^4_{L^4(\Omega)}$.

According to Remark 3.1, u_h is not determined uniquely in general. Moreover, λ_h is not necessarily the smallest eigenvalue of the corresponding discrete eigenvalue

problem. In what follows, u_h refers to an arbitrary solution of Problem 3.2. It will serve as a reference to compare further (cheaper) numerical approximations with. The accuracy of u_h has been studied in [13]. Under the assumption of sufficient regularity, optimal orders of convergence are obtained (cf. (4.5)).

3.2. Preprocessing motivated by numerical homogenization. The aim of this paper is to accurately approximate the fine scale reference solution u_h of Problem 3.2 within some low-dimensional subspace of V_h. For this purpose, we introduce a two-grid upscaling discretization that was initially proposed in [34] for the treatment of multiscale problems. The framework has been applied to nonlinear problems in [27], to linear eigenvalue problems in [33], and in the context of the discontinuous Galerkin [23] and partition of unity methods [28]. This contribution aims to generalize and analyze the methodology to the case of an eigenvalue problem with an additional nonlinearity in the eigenfunction. We emphasize that the coexistence of two difficulties, the nonlinear nature of the eigenproblem itself and the additional nonlinearity in the eigenfunction, requires new essential ideas far beyond simply plugging together existing theories for the isolated difficulties.

Let $\mathcal{N}_H$ denote the set of interior vertices in $\mathcal{T}_H$. For $z \in \mathcal{N}_H$ we let $\Phi_z \in V_H$ denote the corresponding nodal basis function with $\Phi_z(z) = 1$ and $\Phi_z(y) = 0$ for all $y \in \mathcal{N}_H \backslash \{z\}$. We define a weighted Clément-type interpolation operator (cf. [15])

$$(3.2) \quad I_H : H_0^1(\Omega) \to V_H, \quad v \mapsto I_H(v) := \sum_{z \in \mathcal{N}_H} v_z \Phi_z \quad \text{with} \quad v_z := \frac{(v, \Phi_z)_{L^2(\Omega)}}{(1, \Phi_z)_{L^2(\Omega)}}.$$

It is easily shown by Friedrichs' inequality and the Sobolev embedding $H_0^1(\Omega) \hookrightarrow L^6(\Omega)$ (for $d \le 3$) that

$$a(v, \phi) := \int_\Omega A\nabla v \cdot \nabla \phi \, dx + \int_\Omega bv\phi \, dx \qquad \text{for } v, \phi \in H_0^1(\Omega)$$

defines a scalar product in $H_0^1(\Omega)$ and induces a norm $\|\cdot\|_{H^1(\Omega)} := \sqrt{a(\cdot, \cdot)}$ on $H_0^1(\Omega)$ which is equivalent to the standard H^1-norm. By means of the interpolation operator I_H defined in (3.2), we construct an a-orthogonal decomposition of the space V_h into a low-dimensional coarse space $V_{H,h}^c$ (with favorable approximation properties) and a high-dimensional residual space $V_{H,h}^f$. The residual or "fine" space is the kernel of the interpolation operator restricted to V_h,

$$(3.3.\text{a}) \qquad\qquad V_{H,h}^f := \text{kernel}(I_H|_{V_h}).$$

The coarse space is simply defined as the orthogonal complement of $V_{H,h}^f$ in V_h with respect to $a(\cdot, \cdot)$. It is characterized via the a-orthogonal projection $P^f : H_0^1(\Omega) \to V_{H,h}^f$ onto the fine space given by

$$a(P^f v, \phi) = a(v, \phi) \quad \text{for all } \phi \in V_{H,h}^f.$$

By defining $P^c := 1 - P^f$, the coarse space is given by

$$(3.3.\text{b}) \qquad\qquad V_{H,h}^c := P^c V_H.$$

A basis of $V_{H,h}^c$ is given by $(P^c\Phi_z)_{z \in \mathcal{N}_H}$ with $\dim V_{H,h}^c = \dim V_H$. With this definition we obtain the splitting

$$(3.3.\text{c}) \qquad\qquad V_h = V_{H,h}^c \oplus V_{H,h}^f.$$

Some favorable properties of the decomposition, in particular its L^2-quasi-orthogonality, are discussed in section 6.2. The minimization problem in the low-dimensional space $V_{H,h}^c$ reads as follows.

Problem 3.3 (preprocessed approximation). Find $u_H^c \in V_{H,h}^c$ with $(u_H^c, 1) \geq 0$. $\|u_H^c\|_{L^2(\Omega)} = 1$, and

$$E(u_H^c) = \inf_{\substack{v^c \in V_{H,h}^c \\ \|v^c\|_{L^2(\Omega)}=1}} E(v^c).$$

The corresponding eigenvalue in $V_{H,h}^c$ is given by $\lambda_H^c := 2E(u_H^c) + 2^{-1}\beta\|u_H^c\|_{L^4(\Omega)}^4$.

Remark 3.4 (practical aspects of the decomposition).

(a) The assembly of the corresponding finite element matrices requires only the evaluation of $P^f\Phi_z$, i.e., the solution to one linear Poisson-type problem per coarse vertex. This can be done in parallel. Section 3.3 below will show that these linear problems may be restricted to local subdomains centered around the coarse vertices without loss of accuracy. Hence, even in a serial computing setup, the complexity of solving all corrector problems is equivalent (up to factor $|\log(H)|$) to the cost of solving one linear Poisson problem on the fine mesh.

(b) The preprocessing step is independent of the parameter β which characterizes the species of the bosons. Hence, the method becomes considerably cheaper when experiments need to be carried out for different types and numbers of bosons. A similar argument applies to variations on the trapping potential b. Provided that this trapping potential is an element of $H^1(\Omega)$ (in practical applications it is usually even harmonic and admits the desired regularity) the bilinear form $a(\cdot, \cdot)$ (and the associated constructions of $V_{H,h}^f$ and $V_{H,h}^c$) can be restricted to the second order term $\int_\Omega A\nabla v \cdot \nabla\phi$ without a loss in the expected convergence rates stated in Theorems 4.1 and 4.2 below. The trapping potential may then be varied without affecting the pre-processed space $V_{H,h}^c$.

(c) Once the coarse space has been assembled it can also be reused in computations of larger eigenvalues (i.e., not only in the ground state solution).

3.3. Sparse approximations of $V_{H,h}^c$. The construction of the coarse space $V_{H,h}^c$ is based on fine scale equations formulated on the whole domain Ω, which makes them expensive to compute. However, [34] shows that $P^f\Phi_z$ decays exponentially fast away from z. We specify this feature as follows. Let $k \in \mathbb{N}$ denote the localization parameter, i.e., a new discretization parameter. We define nodal patches $\omega_{z,k}$ of k coarse grid layers centered around the node $z \in \mathcal{N}_H$ by

(3.4)
$$\omega_{z,1} := \operatorname{supp}\Phi_z = \cup\{T \in \mathcal{T}_H \mid z \in T\},$$
$$\omega_{z,k} := \cup\{T \in \mathcal{T}_H \mid T \cap \omega_{z,k-1} \neq \emptyset\} \quad \text{for } k \geq 2.$$

There exists $0 < \theta < 1$ depending on the contrast $\gamma_{\min}/\gamma_{\max}$ but not on mesh sizes h, H and fast oscillations of A such that for all vertices $z \in \mathcal{N}_H$ and for all $k \in \mathbb{N}$, it holds that

(3.5)
$$\|P^f\Phi_z\|_{H^1(\Omega\setminus\omega_{z,k})} \lesssim \theta^k\|P^f\Phi_z\|_{H^1(\Omega)}.$$

This result motivates the truncation of the computations of the basis functions to local patches $\omega_{z,k}$. We approximate $\Psi_z = P^f \Phi_z \in V^f_{H,h}$ from (3.3.a)–(3.3.c) with $\Psi_{z,k} \in V^f_{H,h}(\omega_{z,k}) := \{v \in V^f_{H,h} \mid v|_{\Omega \setminus \omega_{z,k}} = 0\}$ such that

$$(3.6) \qquad a(\Psi_{z,k}, v) = a(\Phi_z, v) \quad \text{for all } v \in V^f_{H,h}(\omega_{z,k}).$$

This yields a modified coarse space $V^c_{H,h,k}$ with a local basis

$$(3.7) \qquad V^c_{H,h,k} = \operatorname{span}\{\Phi_z - \Psi_{z,k} \mid z \in \mathcal{N}_H\}.$$

The number of nonzero entries of the corresponding finite element matrices is proportional to $k^d N_H$. (Note that we expect N_H^2 nonzero entries without the truncation.) Due to the exponential decay, the very weak condition $k \approx |\log H|$ implies that the perturbation of the ideal method due to this truncation is of higher order and forthcoming error estimates in Theorems 4.1 and 4.2 remain valid. We refer to [34] for details and proofs. The modified localization procedure from [29] with improved accuracy and stability properties may also be applied.

3.4. Postprocessing. Although u^c_H and λ^c_H will turn out to be highly accurate approximations of the unknown solution (u, λ), the orders of convergence can be improved even further by a simple postprocessing step on the fine grid. The postprocessing applies the two-grid method originally introduced by Xu and Zhou [42] for linear elliptic eigenvalue problems to the present equation by using our upscaled coarse space on the coarse level.

Problem 3.5 (postprocessed approximation). Find $u^c_h \in V_h$ with

$$\int_\Omega A \nabla u^c_h \cdot \nabla \phi_h \, dx + \int_\Omega b u^c_h \phi_h \, dx = \lambda^c_H \int_\Omega u^c_H \phi_h \, dx - \int_\Omega \beta |u^c_H|^2 u^c_H \phi_h \, dx$$

for all $\phi_h \in V_h$. Define $\lambda^c_h := (2E(u^c_h) + 2^{-1}\beta \|u^c_h\|^4_{L^4(\Omega)}) \|u^c_h\|^{-2}_{L^2(\Omega)}$. Let us emphasize that this approach is different from [18], where the postprecessing problem has a different structure and where classical finite element spaces are used on both scales.

4. A-priori error estimates. This section presents the a priori error estimates for the preprocessed/upscaled approximation with and without the postprocessing step. Throughout this section, $u \in H^1_0(\Omega)$ denotes the solution of Problem 2.1, $u_h \in V_h$ the solution of reference Problem 3.2, $u^c_H \in V^c_{H,h}$ the solution of Problem 3.3, and u^c_h the postprocessed solution of Problem 3.5. The notation $f \lesssim g$ abbreviates $f \leq Cg$ with some constant C that may depend on the space dimension d, Ω, $\gamma_{\min}$, $\gamma_{\max}$, $\|b\|_{L^2(\Omega)}$, β, λ and interior angles of the triangulations, but not on the mesh sizes H and h. In particular it is robust against fast oscillations of A and b.

THEOREM 4.1 (error estimates for the preprocessed approximation). *Assume that $\|u - u_h\|_{H^1(\Omega)} \lesssim 1$. For u and u^c_H as above, it holds that*

$$(4.1) \qquad \|u - u^c_H\|_{H^1(\Omega)} \lesssim H^2 + \|u - u_h\|_{H^1(\Omega)}.$$

For sufficiently small h (in the sense of Cancès, Chakir, and Maday et al. [13]), we also have

$$(4.2) \qquad |\lambda - \lambda^c_H| + \|u - u^c_H\|_{L^2(\Omega)} \lesssim H^3 + H \|u - u_h\|_{H^1(\Omega)}.$$

Proof. The proof is postponed to section 6.3. $\square$

The additional postprocessing improves, roughly speaking, the order of accuracy by one.

THEOREM 4.2 (error estimates for the postprocessed approximation). *Assume that h is sufficiently small. The postprocessed approximation u_h^c and the postprocessed eigenvalue λ_h^c satisfy*

$$(4.3) \qquad \|u - u_h^c\|_{H^1(\Omega)} \lesssim H^3 + \|u - u_h\|_{H^1(\Omega)},$$

$$(4.4) \qquad |\lambda - \lambda_h^c| + \|u - u_h^c\|_{L^2(\Omega)} \lesssim H^4 + C_{L^2}(h, H).$$

The constant $C_{L^2}(h, H)$ behaves roughly like $H^2\|u - u_h\|_{H^1(\Omega)}$ and can be extracted from the proofs in section 6.4.2.

Proof. The proof is postponed to section 6.4. ☐

Let us emphasize that both theorems remain valid for $V_{H,h}^c$ replaced with its sparse approximation $V_{H,h,k}^c$ (cf. section 3.3) for moderate localization parameter $k \gtrsim |\log H|$.

We shall discuss the behavior of the fine scale errors $u - u_h$ and $\lambda - \lambda_h$. Recall from [13] that for a bounded domain Ω with polygonal Lipschitz boundary, $A \in [W^{1,\infty}(\Omega)]^{d \times d}$, and sufficiently small h, the fine scale error $\|u - u_h\|_{H^1(\Omega)}$ satisfies the optimal estimate

$$(4.5) \qquad \|u - u_h\|_{H^1(\Omega)} + h^{-1}\|u - u_h\|_{L^2(\Omega)} + h^{-1}|\lambda - \lambda_h| \lesssim h.$$

The proof in [13] is for constant $A = 1$ and hyperrectangle Ω but it is easily checked that the estimates remain valid for any bounded domain Ω with polygonal Lipschitz boundary and $A \in [W^{1,\infty}(\Omega)]^{d \times d}$. Under these assumptions our a priori estimates for the postprocessed approximation of the ground state eigenvalue summarize as follows:

$$|\lambda - \lambda_h^c| \lesssim H^4 + H^2 h.$$

Hence, in this regular setting, the choice $H = h^{1/2}$ ensures that the loss of accuracy is negligible when compared to the accuracy of the expensive full fine scale approximation λ_h. However, with regard to the numerical experiment in section 5.1 below, this choice might be pessimistic.

Moreover, note that the fine scale error depends crucially on higher Sobolev regularity of the solution, whereas our estimates for the coarse scale error require only minimal regularity that holds under assumptions (a)–(d) in section 2. Thus, we believe that in a less regular setting, even coarser choices of H relative to h will balance the discretization errors on the coarse and the fine scale.

5. Numerical experiments. Any numerical approach for the computation of ground states of a BEC involves an iterative algorithm that starts with a given initial value and diminishes the energy of the density functional E in each iteration step. In this contribution, we use the optimal damping algorithm (ODA) originally developed by Cancès and Le Bris [14, 12] for the Hartree–Fock equations, since it suits our preprocessing framework. The ODA involves solving a linear eigenvalue problem in each iteration step. However, after preprocessing, these linear eigenvalue problems are very low dimensional and the precomputed basis of $V_{H,h}^c$ can be reused for each of these problems, making the iterations extremely cheap. The approximations produced by the ODA are known to rapidly converge to a solution of the discrete minimization problem. (See [21] and [12] for a proof in the setting of the Hartree–Fock equations.) All subsequent numerical experiments have been performed using MATLAB.

5.1. Numerical results for harmonic potential. In this section, we choose the smooth experimental setup of [13, section 4, p. 109; Figure 2], i.e., $\Omega := (0, \pi)^2$, $b(x_1, x_2) := x_1^2 + x_2^2$, $A = 1$, $\beta = 1$ and with homogeneous Dirichlet boundary condition. Our method depends basically on three parameters: the coarse mesh size H, the fine mesh size h, and the localization parameter k (cf. section 3.3 and [29]). In all computations of this section we couple k to the coarse mesh size by choosing $k = 2 \log_2 H$. This choice is made such that the error of localization is negligible when compared with the errors committed by the fine scale discretization and the upscaling. All approximations are computed with the ODA method as presented in [21, section 2] with accuracy parameter $\varepsilon_{\mathrm{ODA}} = 10^{-14}$.

5.1.1. Comparison with full fine scale approximation. In the first experiment, we consider uniform coarse meshes $\mathcal{T}_H$ with mesh width parameters $H = 2^{-1}\pi, 2^{-2}\pi, \ldots, 2^{-4}\pi$ of Ω. The fine mesh $\mathcal{T}_h$ for the pre- and postprocessing has width $h = 2^{-7}\pi$ and remains fixed. We study the error committed by coarsening from a fine scale h to several coarse scales H, i.e., we study the distance between the ground state (u_h, λ_h) of Problem 3.2 and either the coarse scale approximation (u_H^c, λ_H^c) of Problem 3.3 (with underlying fine scale h) or its postprocessed version (u_h^c, λ_h^c) of Problem 3.5. Our theoretical results do not allow predictions about the coarsening error. Most likely, this is an artifact of our theory and we conjecture that (u_h, λ_h) and its coarse approximations (u_H^c, λ_H^c) and (u_h^c, λ_h^c) are in fact super-close in the sense of

$$(5.1) \qquad H^{-1}\|u_h - u_H^c\|_{H^1(\Omega)} + \|u_h - u_H^c\|_{L^2(\Omega)} + |\lambda_h - \lambda_H^c| \lesssim H^3,$$
$$H^{-1}\|u_h - u_h^c\|_{H^1(\Omega)} + \|u_h - u_h^c\|_{L^2(\Omega)} + |\lambda_h - \lambda_h^c| \lesssim H^4.$$

This assertion is true in the limit $h \to 0$. Section 5.1.2 supports numerically the assertion for positive h. Figure 1 reports the numerical results. Observe that the

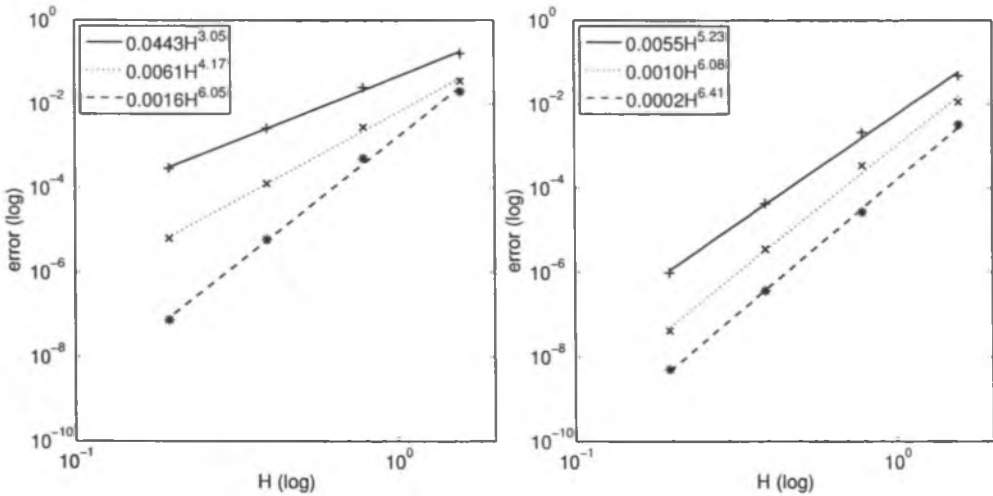FIG. 1. *Results for harmonic potential. Left: Errors of preprocessed approximation $\|u_h - u_H^c\|_{H^1(\Omega)}$ (+), $\|u_h - u_H^c\|_{L^2(\Omega)}$ (×), and $|\lambda_h - \lambda_H^c|$ (∗) versus coarse mesh size H. Right: Errors of postprocessed approximation $\|u_h - u_h^c\|_{H^1(\Omega)}$ (+), $\|u_h - u_h^c\|_{L^2(\Omega)}$ (×), and $|\lambda_h - \lambda_h^c|$ (∗) versus coarse mesh size H.*

experimental rates with respect to H displayed in the figures are in fact better than the rates indicated by Theorems 4.1–4.2 and conjectured in (5.1). The reason could be the high regularity of the underlying (exact) solution $u \in H^3(\Omega)$. We do not exploit additional regularity in our error analysis. Similar observations have been made for the linear eigenvalue problem: see [33, Remark 3.3] for details and some justification of higher rates under additional regularity assumptions. Our implementation is not yet adequate for a fair comparison with regard to computational complexity and computing times between standard fine scale finite elements and our two-level techniques. However, to convince the reader of the potential savings in our new approach, let us mention that the number of iterations of the ODA was basically the same for both approaches in all numerical experiments. This statement applies as well to more challenging setups with larger values of β (see, e.g., section 5.2 below), where ODA needs many iterations to fall below some prescribed tolerance. We thus conclude that the actual speed-up of our approach is truly reflected by the dimension reduction from h^{-d} to H^{-d} up to the overhead $\mathcal{O}(k) = \mathcal{O}(\log|H|)$ induced by slightly denser (but still sparse) finite element matrices on the coarse level.

5.1.2. Comparison with high-resolution numerical approximation. In the second experiment we investigate the role of the fine scale parameter h. We consider uniform coarse meshes $\mathcal{T}_H$ with mesh width parameters $H = 2^{-1}\pi, \ldots, 2^{-3}\pi$ and uniform fine meshes $\mathcal{T}_h$ for $h = H/4, \ldots, 2^{-7}\pi$ for pre- and postprocessing computations. The error between the exact eigenvalue λ and coarse approximations λ_H^c and λ_h^c is estimated via a high-resolution numerical solution on a mesh of width $2^{-9}\pi$. The results are reported in Figure 2. For clarity, we show eigenvalue errors only. We conclude that it would have been sufficient to choose $H \approx h^{1/3}$ to achieve the accuracy of λ_h by our coarse approximation scheme with postprocessing.
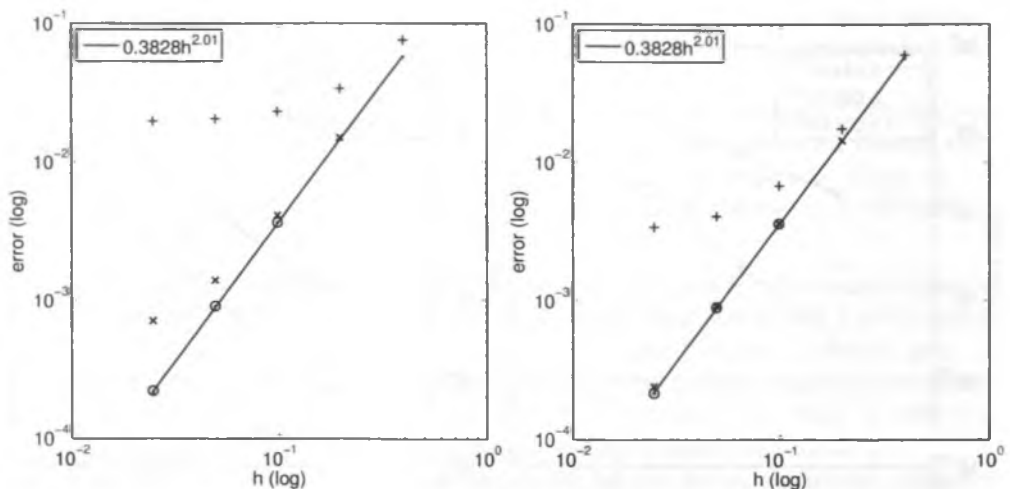
FIG. 2. *Results for harmonic potential. Left: (estimated) errors of preprocessed approximation* $|\lambda - \lambda_H^c|$ *for fixed values* $H = 2^{-1}\pi$ *(+),* $H = 2^{-2}\pi$ *(×), and* $H = 2^{-3}\pi$ *(○) versus fine mesh size* h. *Right: (estimated) errors of postprocessed approximation* $|\lambda - \lambda_h^c|$ *for fixed values* $H = 2^{-1}\pi$ *(+),* $H = 2^{-2}\pi$ *(×), and* $H = 2^{-3}\pi$ *(○) versus fine mesh size* h. *In both plots, the (estimated) error of the standard FEM on the fine mesh* $|\lambda - \lambda_h|$ *(●) is depicted for reference.*
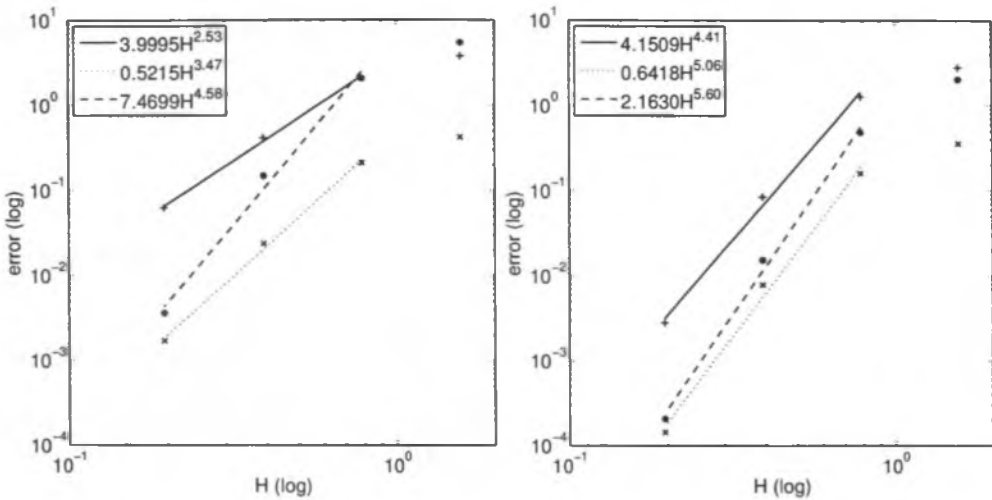
FIG. 3. *Results for periodic potential. Left: Errors of preprocessed approximation* $\|u_h - u_H^c\|_{H^1(\Omega)}$ *(+),* $\|u_h - u_H^c\|_{L^2(\Omega)}$ *(×), and* $|\lambda_h - \lambda_H^c|$ *(*) versus coarse mesh size H. Right: Errors of postprocessed approximation* $\|u_h - u_h^c\|_{H^1(\Omega)}$ *(+),* $\|u_h - u_h^c\|_{L^2(\Omega)}$ *(×), and* $|\lambda_h - \lambda_h^c|$ *(*) versus coarse mesh size H.*

5.2. Numerical results for discontinuous periodic potential. This section addresses the case of a BEC that is trapped in a periodic potential. Periodic potentials are of special interest since they can be used to explore physical phenomena such as Josephson oscillations and macroscopic quantum self-trapping of the condensate (cf. [41, 43]). Here we use a potential b that describes a periodic array of quantum wells that can be experimentally generated by the interference of overlapping laser beams (cf. [39]).

Let $\Omega = (0, \pi)^2$, $A = 1$, and $\beta = 4$. Given $b_t = 100$ and $L = 4$, define

$$b_0(x_1, x_2) := \begin{cases} 0 & \text{for } x \in \left]\frac{1}{4}, \frac{3}{4}\right[^2, \\ b_t & \text{else} \end{cases}$$

and the potential $b(x) = b_0\big(L\big(x/\pi - \frac{\lfloor Lx/\pi\rfloor}{L}\big)\big)$.

Consider the same numerical setup as in section 5.1.1 (i.e., we draw our attention again to the coarsening error $u_h - u_H^c$) with the exception that we were able to reduce the localization parameter $k = \log_2 H$ without affecting the best convergence rates possible. Figure 3 reports the errors between the fine scale reference discretization and our coarse approximations. For the discontinuous potential, the experimental rates (with respect to H) are slightly worse than those ones observed in section 5.1.1. However, they are still better than the rates indicated by Theorems 4.1–4.2 and conjectured in (5.1).

6. Proofs of the main results. In this section we are concerned with proving the main theorems.

6.1. Auxiliary results. An application of [13, Theorem 1] shows that u_h and u_H^c both converge to u in $H^1(\Omega)$, which guarantees stability.

Remark 6.1 (stability of discrete approximations). For sufficiently small h we have

(6.1) $$\|u_h\|_{H^1(\Omega)} \leq \sqrt{\lambda_h} \lesssim \sqrt{\lambda} \qquad \text{and}$$

(6.2) $$\|u_h\|_{L^4(\Omega)} \leq \left(\frac{\lambda_h}{\beta}\right)^{\frac{1}{4}} \lesssim \left(\frac{\lambda}{\beta}\right)^{\frac{1}{4}}.$$

The same results hold for u_h replaced by u_H^c and λ_h replaced by λ_H^c for h and H sufficiently small.

The bound (6.1) is obvious using $\|u_h\|_{L^2(\Omega)} = 1$ and the H^1-convergence $u_h \to u$ which guarantees $\lambda_h \to \lambda$. Estimate (6.2) directly follows from the definitions of λ_h and E_h which gives us $\lambda_h \geq 2E(u_h) = a(u_h, u_h) + \frac{\beta}{2}\|u_h\|_{L^4(\Omega)}^4 \geq \frac{\beta}{2}\|u_h\|_{L^4(\Omega)}^4$.

Remark 6.2 (L^∞-bound). The solution u of Problem 2.1 is in $L^\infty(\Omega)$. This follows from the uniqueness of $u \in H_0^1(\Omega)$, which shows that it is also the unique solution of the linear elliptic problem

$$\int_\Omega A\nabla u \cdot \nabla \phi + bu\phi \, dx = \int_\Omega \bar{f}\phi \, dx \qquad \text{for all } \phi \in H_0^1(\Omega),$$

where $\bar{f} := (\lambda u - \beta|u|^3) \in L^2(\Omega)$. Standard theory for linear elliptic problems (cf. [25, Theorem 8.15, pp. 189–193]) then yields the existence of a constant c only depending on Ω, d and $\|\gamma_{\min}^{-1}b\|_{L^2(\Omega)}$ such that

(6.3) $$\|u\|_{L^\infty(\Omega)} \leq c(\|u\|_{L^2(\Omega)} + \gamma_{\min}^{-1}\|\bar{f}\|_{L^2(\Omega)}) \lesssim 1 + \|u\|_{L^6(\Omega)}^3 \lesssim 1 + \|u\|_{H^1(\Omega)}^3.$$

6.2. Properties of the coarse space $V_{H,h}^c$. Recall the local approximation properties of the weighted Clément-type interpolation operator I_H defined in (3.2),

(6.4) $$H_T^{-1}\|v - I_H(v)\|_{L^2(T)} + \|\nabla(v - I_H(v))\|_{L^2(T)} \leq C_{I_H}\|\nabla v\|_{L^2(\omega_T)}$$

for all $v \in H_0^1(\Omega)$. Here, C_{I_H} is a generic constant that depends only on interior angles of $\mathcal{T}_H$ but not on the local mesh size and $\omega_T := \bigcup\{S \in \mathcal{T}_H | \overline{S} \cap \overline{T} \neq \emptyset\}$. Furthermore, for all $v \in H_0^1(\Omega)$ and for all $z \in \mathcal{N}_H$ it holds that

(6.5) $$\int_{\omega_z} (v - v_z)^2 \, dx \leq C_{I_H} H^2 \|\nabla v\|_{L^2(\omega_z)}^2,$$

where $\omega_z := \operatorname{supp}(\Phi_z)$ and v_z is given by (3.2).

LEMMA 6.3 (properties of the decomposition). *The decomposition of V_h into V_H and $V_{H,h}^f$ (stated in section 3.2) is L^2-orthogonal, i.e.,*

(6.6) $$V_h = V_H \oplus V_{H,h}^f \quad and \quad (v_H, v^f)_{L^2(\Omega)} = 0 \text{ for all } v_H \in V_H, \ v^f \in V_{H,h}^f.$$

The decomposition of V_h in $V_{H,h}^c$ and $V_{H,h}^f$ is a-orthogonal

(6.7) $$V_h = V_{H,h}^c \oplus V_{H,h}^f \quad and \quad a(v^c, v^f) = 0 \text{ for all } v^c \in V_{H,h}^c, \ v^f \in V_{H,h}^f$$

and L^2-quasi-orthogonal in the sense that

(6.8) $$(v^c, v^f)_{L^2(\Omega)} \lesssim H^2\|\nabla v^c\|_{L^2(\Omega)}\|\nabla v^f\|_{L^2(\Omega)}.$$

Proof. The proof is verbatim the same as in [33]. □

The following lemma estimates the error of the best approximation in the modified coarse space $V_{H,h}^c$. The lemma is also implicitly required each time that we use the abstract error estimates stated in [13, Theorem 1]. These estimates require a family of finite dimensional spaces that is dense in $H_0^1(\Omega)$. This density property is implied by the following lemma.

LEMMA 6.4 (approximation property of $V_{H,h}^c$). *For any given $v \in H_0^1(\Omega)$ with* div $A\nabla v \in L^2(\Omega)$ *it holds that*

$$\inf_{v_H^c \in V_{H,h}^c} \|v - v_H^c\|_{H^1(\Omega)} \lesssim H \| \operatorname{div} A\nabla v + bv\|_{L^2(\Omega)} + \inf_{v_h \in V_h} \|v - v_h\|_{H^1(\Omega)}.$$

Proof. Given v, define $f_v := \operatorname{div} A\nabla v + bv \in L^2(\Omega)$ (since $v \in L^\infty(\Omega)$) and let $v_h \in V_h$ denote the corresponding finite element approximation, i.e.,

$$a(v_h, \phi_h) = (f_v, \phi_h)_{L^2(\Omega)} \qquad \text{for all } \phi_h \in V_h.$$

With $v_H^c := P^c v_h \in V_{H,h}^c$, Galerkin orthogonality leads to

$$\|A^{1/2}\nabla(v_h - v_H^c)\|_{L^2(\Omega)}^2 \overset{(6.7)}{\leq} a(v_h, P^f v_h) = (f_v, P^f v_h)_{L^2(\Omega)}$$
$$\overset{(6.4)}{\lesssim} \gamma_{\min}^{-1/2} \|H f_v\|_{L^2(\Omega)} \|A^{1/2}\nabla(v_h - v_H^c)\|_{L^2(\Omega)}.$$

This, the triangle inequality, and norm equivalences readily yield the assertion. □

Next, we show that there exists an element $u^c = P^c u_h$ in the space $V_{H,h}^c$ that approximates u_h in the energy norm with an accuracy of order $O(H^2)$.

LEMMA 6.5 (stability and approximability of the reference solution). *Let $(u_h, \lambda_h) \in V_h \times \mathbb{R}$ solve Problem* 3.2. *Then it holds that*

$$\|P^c u_h\|_{H^1(\Omega)} \leq \sqrt{\lambda_h},$$
$$\|P^c u_h - u_h\|_{H^1(\Omega)} = \|P^f u_h\|_{H^1(\Omega)} \lesssim H^2 + H\|u - u_h\|_{H^1(\Omega)},$$
$$(P^c u_h, P^f u_h)_{L^2(\Omega)} \lesssim \left(H^2 + H\|u - u_h\|_{H^1(\Omega)} \right) H^2.$$

Proof. Recall $\| \cdot \|_{H^1(\Omega)} := \sqrt{a(\cdot, \cdot)}$. Since P^c is a projection, we have

$$\|P^c u_h\|_{H^1(\Omega)}^2 \leq \|u_h\|_{H^1(\Omega)}^2 = \lambda_h \|u_h\|_{L^2(\Omega)}^2 - \beta\|u_h\|_{L^4(\Omega)}^4 \leq \lambda_h.$$

The a-orthogonality of (3.3.c) further yields

$$(6.9) \qquad \|P^f u_h\|_{H^1(\Omega)}^2 = a(P^f u_h, P^f u_h) = a(u_h, P^f u_h)$$
$$= \lambda_h(u_h, (1 - I_H)P^f u_h)_{L^2(\Omega)} - \beta(u^3, P^f u_h)_{L^2(\Omega)}$$
$$- \beta(u_h^3 - u^3, P^f u_h)_{L^2(\Omega)}.$$

The first term on the right-hand side of (6.9) can be bounded using $I_H(P^f u_h) = 0$, the L^2-orthogonality (6.6), and the estimates for the weighted Clément interpolation operator (6.4)

$$(6.10) \qquad \lambda_h(u_h, (1 - I_H)P^f u_h)_{L^2(\Omega)} = \lambda_h((1 - I_H)u_h, (1 - I_H)P^f u_h)_{L^2(\Omega)}$$
$$\lesssim \lambda_h H^2 \|u_h\|_{H^1(\Omega)} \|P^f u_h\|_{H^1(\Omega)}.$$

Since $u \in L^{\infty}(\Omega)$ we have $\nabla(u^3) = 3u^2\nabla u \in L^2(\Omega)$ and, hence, the second term on the right-hand side of (6.9) can be bounded as follows:

(6.11)

$$\beta(u^3, P^f u_h) = \beta((1 - I_H)u^3, (1 - I_H)P^f u_h) \overset{(6.5)}{\lesssim} H^2 \|u\|_{L^\infty(\Omega)}^2 \|u\|_{H^1(\Omega)} \|P^f u\|_{H^1(\Omega)}$$

$$\overset{(6.3)}{\lesssim} H^2 \|u\|_{H^1(\Omega)} \|P^f u\|_{H^1(\Omega)}.$$

Since $u_h^3 - u^3 = (u_h^2 + u_h u + u^2)(u_h - u)$, the third term on the right-hand side of (6.9) can be estimated by

(6.12) $\beta(u_h^3 - u^3, P^f u_h)_{L^2(\Omega)} \lesssim \||u| + |u_h|\|_{L^6(\Omega)}^2 \|u_h - u\|_{L^6(\Omega)} \|(1 - I_H)P^f u_h\|_{L^2(\Omega)}$

$$\lesssim H\|u - u_h\|_{H^1(\Omega)} \|P^f u_h\|_{H^1(\Omega)},$$

where we used (6.1) and the embedding $\||u| + |u_h|\|_{L^6(\Omega)} \lesssim \|u\|_{H^1(\Omega)} + \|u_h\|_{H^1(\Omega)}$.

The combination of (6.9)–(6.12) readily yields

$$\|P^f u_h\|_{H^1(\Omega)} \lesssim H^2 + \|u - u_h\|_{H^1(\Omega)}^2.$$

The third assertion follows from the previous ones and

$$(P^c u_h, P^f u_h)_{L^2(\Omega)} = ((1 - I_H)P^c u_h, (1 - I_H)P^f u_h)_{L^2(\Omega)}$$

$$\lesssim H^2 \|P^c u_h\|_{H^1(\Omega)} \|P^f u_h\|_{H^1(\Omega)}. \qquad \square$$

6.3. Proof of Theorem 4.1. We split the proof into two parts: the estimate for the H^1-error and the estimate for the L^2-error.

6.3.1. Proof of the H^1-error estimate (4.1). We proceed similarly as in [13]. The proof is divided into four steps. In the first step, we derive an identical formulation of some energy difference. The identity is used in Step 2 to establish the inequality $\|u_h^c - u\|_{H^1(\Omega)}^2 \lesssim E(u_h^c) - E(u)$. Since u_h^c is a minimizer, we can replace $E(u_h^c)$ by $E(w_h^c)$ in the estimate for an arbitrary L^2-normalized $w_h^c \in V_{H,h}^c$. In Step 3, we choose $w_h^c := \frac{P^c u_h}{\|P^c u_h\|_{L^2(\Omega)}}$ and show that the perturbation introduced via normalization is of high order ($\approx H^3$). In Step 4, we use Step 3 to estimate $E(w_h^c) - E(u)$.

Step 1. Given some arbitrary $w \in H_0^1(\Omega)$ with $\|w\|_{L^2(\Omega)} = 1$, we show that

(6.13) $\quad E(w) - E(u) = \frac{1}{2}a(w - u, w - u) + \frac{\beta}{2}(|u|^2(w - u), w - u)_{L^2(\Omega)}$

$$+ \frac{\beta}{4}((|u|^4 - 2|u|^2|w|^2 + |w|^4, 1)_{L^2(\Omega)} - \frac{1}{2}\lambda\|w - u\|_{L^2(\Omega)}^2.$$

First, using $\|u\|_{L^2(\Omega)} = \|w\|_{L^2(\Omega)} = 1$ we get

(6.14) $\qquad \lambda(u - w, u - w)_{L^2(\Omega)} = \lambda\|u\|_{L^2(\Omega)}^2 - 2\lambda(u, w)_{L^2(\Omega)} + \lambda\|u\|_{L^2(\Omega)}^2$

$$= -2\lambda(u, w - u)_{L^2(\Omega)}$$

$$= -2a(u, w - u) - 2\beta(|u|^2 u, w - u)_{L^2(\Omega)}.$$

This yields

$$
\begin{aligned}
&a(w,w) + \beta(|u|^2 w, w)_{L^2(\Omega)} - a(u,u) - \beta(|u|^2 u, u)_{L^2(\Omega)} \\
&\overset{(6.14)}{=} \quad a(w,w) - 2a(u,w) + a(u,u) \\
&\qquad + \beta(|u|^2 w, w)_{L^2(\Omega)} - 2\beta(|u|^2 u, w)_{L^2(\Omega)} + \beta(|u|^2 u, u)_{L^2(\Omega)} \\
&\qquad - \lambda(w-u, w-u)_{L^2(\Omega)} \\
&= \quad a(w-u, w-u) + \beta(|u|^2(w-u), w-u)_{L^2(\Omega)} - \lambda\|w-u\|^2_{L^2(\Omega)}.
\end{aligned}
$$

Plugging this last equality into the equation

$$
2E(w) - 2E(u) = a(w,w) + \frac{\beta}{2}(|w|^2 w, w)_{L^2(\Omega)} - a(u,u) - \frac{\beta}{2}(|u|^2 u, u)_{L^2(\Omega)}
$$

leads to (6.13).

Step 2. Using (6.13) with $w = u_h^c$ and the fact that there exists some c_0 (independent of H and h) such that $a(u - u_h^c, u - u_h^c) + ((\beta|u|^2 - \lambda)(u - u_h^c), u - u_h^c)_{L^2(\Omega)} \geq c_0\|u - u_h^c\|^2_{H^1(\Omega)}$ (cf. [13, Lemma 1]), we get

$$
\begin{aligned}
E(u_h^c) - E(u) &= \frac{1}{2}a(u_h^c - u, u_h^c - u) + \frac{\beta}{2}(|u|^2(u_h^c - u), u_h^c - u)_{L^2(\Omega)} \\
&\qquad + \frac{\beta}{4}(|u|^4 - 2|u|^2|u_h^c|^2 + |u_h^c|^4, 1)_{L^2(\Omega)} - \frac{1}{2}\lambda\|u_h^c - u\|^2_{L^2(\Omega)} \\
&\geq \frac{c_0}{2}\|u_h^c - u\|^2_{H^1(\Omega)} + \frac{\beta}{4}\||u|^2 - |u_h^c|^2\|^2_{L^2(\Omega)}.
\end{aligned}
$$

Step 3. Using the result of step two yields

$$
\|u_h^c - u\|^2_{H^1(\Omega)} \lesssim E(u_h^c) - E(u) \leq E(w_h^c) - E(u)
$$

for any L^2-normalized $w_h^c \in V_{H,h}^c$. We choose $w_h^c := \frac{P^c u_h}{\|P^c u_h\|_{L^2(\Omega)}}$ and observe that we get, with Lemma 6.5, that

(6.15)
$$
\begin{aligned}
\|P^c u_h - w_h^c\|_{L^2(\Omega)} &= \big|1 - \|P^c u_h\|_{L^2(\Omega)}\big| \leq \|P^f u_h\|_{L^2(\Omega)} = \|P^f u_h - I_H(P^f u_h)\|_{L^2(\Omega)} \\
&\lesssim H\|P^f u_h\|_{H^1(\Omega)} \lesssim H\|u - u_h\|^2_{H^1(\Omega)} + H^3
\end{aligned}
$$

and consequently

(6.16)
$$
\|P^c u_h - w_h^c\|_{H^1(\Omega)} = \frac{\big|1 - \|P^c u_h\|_{L^2(\Omega)}\big|}{\|P^c u_h\|_{L^2(\Omega)}}\|P^c u_h\|_{H^1(\Omega)} \lesssim H\|u - u_h\|^2_{H^1(\Omega)} + H^3,
$$

where we used $\|u - u_h\|_{H^1(\Omega)} \lesssim 1$ (implying $\|P^c u_h\|_{H^1(\Omega)} \lesssim 1$ and $\|P^c u_h\|_{L^2(\Omega)} \gtrsim 1$).

Step 4. Using again (6.13) leads to

$$
\begin{aligned}
2E(w_h^c) - 2E(u) &= \|w_h^c - u\|^2_{H^1(\Omega)} + \beta(|u|^2(w_h^c - u), w_h^c - u)_{L^2(\Omega)} \\
&\qquad + \frac{\beta}{2}(|u|^4 - 2|u|^2|w_h^c|^2 + |w_h^c|^4, 1)_{L^2(\Omega)} - \lambda\|w_h^c - u\|^2_{L^2(\Omega)}.
\end{aligned}
$$

The Hölder inequality

$$(6.17) \qquad (|u|^2, |u - w_h^c|^2)_{L^2(\Omega)} \le \|u\|_{L^6(\Omega)}^2 \|u - w_h^c\|_{L^2(\Omega)} \|u - w_h^c\|_{L^6(\Omega)}$$

yields the estimate

$$\beta(|u|^2(w_h^c - u), w_h^c - u)_{L^2(\Omega)} + \frac{\beta}{2} \int_\Omega \left(|u|^2 - |w_h^c|^2\right)^2 \, dx$$

$$\stackrel{(6.17)}{\le} \beta\|u\|_{L^6(\Omega)}^2 \|u - w_h^c\|_{L^2(\Omega)} \|u - w_h^c\|_{L^6(\Omega)} + \frac{\beta}{2}((|u| + |w_h^c|)^2, |u - w_h^c|^2)_{L^2(\Omega)}$$

$$\stackrel{(6.17)}{\le} \beta(2\|u\|_{L^6(\Omega)}^2 + \|w_h^c\|_{L^6(\Omega)}^2)\|u - w_h^c\|_{L^2(\Omega)} \|u - w_h^c\|_{L^6(\Omega)}$$

$$\lesssim \|u - w_h^c\|_{L^2(\Omega)}^2 + \|u - w_h^c\|_{H^1(\Omega)}^2$$

for the terms involving β. The combination of the previous results with Lemma 6.5 and estimates (6.15) and (6.16) gives us

$$\|u_h^c - u\|_{H^1(\Omega)}^2 \lesssim E(u_h^c) - E(u) \le E(w_h^c) - E(u) \lesssim \|w_h^c - u\|_{H^1(\Omega)}^2$$

$$\lesssim \|u - P^c u_h\|_{H^1(\Omega)}^2 + \|P^c u_h - w_h^c\|_{H^1(\Omega)}^2$$

$$\lesssim \left(\|u - u_h\|_{H^1(\Omega)} + H^2\right)^2.$$

6.3.2. Proof of the L^2-error estimate (4.2). In the following, we let the bilinear form $c_{\lambda,u} : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ be given by

$$c_{\lambda,u}(v, w) := \int_\Omega A\nabla v \cdot \nabla w + bvw + 3\beta|u|^2 vw \, dx - \lambda \int_\Omega vw \, dx$$

and we define the space

$$V_u^\perp := \{v \in H_0^1(\Omega)| \, (v, u)_{L^2(\Omega)} = 0\}.$$

For $w \in H_0^1(\Omega)$ we let $\psi_w \in V_u^\perp$ denote the unique solution (see Lemma 6.6 below) of

$$(6.18) \qquad c_{\lambda,u}(\psi_w, v_\perp) = (w, v_\perp)_{L^2(\Omega)} \quad \text{for all } v_\perp \in V_u^\perp.$$

The subsequent lemma applies the abstract L^2-error estimate, obtained by Cancès, Chakir, and Maday [13, Lemma 1, Theorem 1, and Remark 2], to our setting. Observe that Lemma 6.4 (i.e., $V_{H,h}^c$ represents a dense family of finite dimensional subspaces of H^1) is required to apply these results.

LEMMA 6.6 (abstract approximation [13]). *Let h be sufficiently small; then*

$$(6.19) \qquad |\lambda - \lambda_H^c| \lesssim \|u - u_H^c\|_{H^1(\Omega)}^2 + \|u - u_H^c\|_{L^2(\Omega)}$$

and

$$(6.20) \qquad \|u - u_H^c\|_{L^2(\Omega)}^2 \lesssim \|u - u_H^c\|_{H^1(\Omega)} \inf_{\psi \in V_{H,h}^c} \|\psi_{u_H^c - u} - \psi\|_{H^1(\Omega)}.$$

Furthermore, the bilinear form $c_{\lambda,u}(\cdot, \cdot)$ is a scalar product in $H_0^1(\Omega)$ and induces a norm that is equivalent to the standard H^1-norm.

Observe the following equivalence. If $\psi_w \in V_u^\perp$ solves

$$\int_\Omega A\nabla\psi_w \cdot \nabla v_\perp + b\psi_w v_\perp + \beta 3|u|^2 \psi_w v_\perp \, dx - \lambda \int_\Omega \psi_w v_\perp \, dx = \int_\Omega wv_\perp \, dx$$

for all $v_\perp \in V_u^\perp$, then it also solves

$$\int_\Omega A\nabla\psi_w \cdot \nabla v + b\psi_w v + \beta 3|u|^2\psi_w v\,dx - \lambda \int_\Omega \psi_w v\,dx$$
$$= 2\beta(u^3, \psi_w)_{L^2(\Omega)} \int_\Omega uv\,dx + \int_\Omega (w - (w,u)_{L^2(\Omega)})v\,dx$$

for all $v \in H_0^1(\Omega)$. This can be easily seen as follows: assume $\operatorname{div} A\nabla\psi_w \in L^2(\Omega)$ (the general result follows by density arguments) and let $P^\perp : L^2(\Omega) \to V_u^\perp$ denote the L^2-orthogonal projection given by $P^\perp(v) := v - (v,u)_{L^2(\Omega)}$. Since

$$\int_\Omega \left(- \operatorname{div} A\nabla\psi_w + b\psi_w + 3\beta|u|^2\psi_w - \lambda\psi_w\right) v^\perp\,dx = \int_\Omega wv^\perp\,dx,$$

we get

$$\int_\Omega P^\perp \left(- \operatorname{div} A\nabla\psi_w + b\psi_w + 3\beta|u|^2\psi_w - \lambda\psi_w\right) v\,dx = \int_\Omega P^\perp(w)v\,dx$$

for all $v \in H_0^1(\Omega)$. By using the explicit formula for $P^\perp$ and the definition of u the reformulated equation follows. Furthermore, since $\psi_w \in H_0^1(\Omega)$ solves a standard elliptic problem, classical theory (cf. [25]) applies and we get the L^∞-estimate

$$(6.21) \quad \|\psi_w\|_{L^\infty(\Omega)} \lesssim (1+\lambda)\|\psi_w\|_{L^2(\Omega)} + |(|u|^3, \psi_w)| + \|w\|_{L^2(\Omega)} \lesssim (1+\lambda)\|w\|_{L^2(\Omega)}.$$

LEMMA 6.7 (L^2-error estimate). *Let h be sufficiently small and let u denote the solution of Problem 2.1, u_H^c the solution of Problem 3.3, and $\psi_{u-u_H^c} \in V_u^\perp$ the solution of (6.18) for $w = u - u_H^c$. Then*

$$\|u - u_H^c\|_{L^2(\Omega)} \lesssim \left(\min_{\psi^h \in V_h} \frac{\|\psi_{u-u_H^c} - \psi^h\|_{H^1(\Omega)}}{\|u - u_H^c\|_{L^2(\Omega)}} + H\right) \|u - u_H^c\|_{H^1(\Omega)}.$$

In Lemma 6.7, the assumption that h should be sufficiently small enters by using the L^2-estimate (6.20). Note that the coarse mesh size H remains unconstrained.

Proof. We define $e_H^c := u - u_H^c$. Using Lemma 6.6 (and therefore implicitly Lemma 6.4) we get

$$(6.22) \quad \frac{\|e_H^c\|_{L^2(\Omega)}^2}{\|e_H^c\|_{H^1(\Omega)}} \lesssim \|\psi_{u-u_H^c} - \psi_H^c\|_{H^1(\Omega)} \leq \|\psi_{u-u_H^c} - \psi^h\|_{H^1(\Omega)} + \|\psi_H^c - \psi^h\|_{H^1(\Omega)}$$

for all $\psi_H^c \in V_{H,h}^c$ and all $\psi^h \in V_h$. It remains to properly choose ψ^h and ψ_H^c. The proof is structured as follows. We choose $\phi_h \in V_h$ to be the fine space approximation of the solution of the adjoint problem (6.18) and ψ_H^c is chosen to be the $a(\cdot, \cdot)$-orthogonal approximation of ψ^h. This guarantees that $\psi_H^c - \psi^h$ is in the kernel of our interpolation operator (i.e., $I_H(\psi_H^c - \psi^h) = 0$) and we can estimate the occurring terms while gaining an additional error order of H. The proof is detailed in the following.

Let us choose $\psi^h := \psi^h_{e^{\cdot}_{II}}$, where $\psi^h_{e^{\cdot}_{II}} \in V_h$ solves

$$c_{\lambda,u}(\psi^h_{e^{\cdot}_{II}}, v_h) = 2\beta(|u|^3, \psi^h_{e^{\cdot}_{II}})_{L^2(\Omega)} \int_\Omega u v_h \, dx + \int_\Omega (e^c_H - (e^c_H, u)_{L^2(\Omega)}) v_h \, dx$$

for all $v_h \in V_h$. The coercivity of $c_{\lambda,u}$ and reinterpretation of the equation in the sense of problem (6.18) yields that $\psi^h_{e^{\cdot}_{II}}$ is well defined. Next, we define

$$g(v, w, u) := -\beta 3|u|^2 v + \lambda v + 2\beta(|u|^3, v)_{L^2(\Omega)} u + (w - (w, u)_{L^2(\Omega)})$$

and solve for $\psi^{H,c}_{e^{\cdot}_{II}} \in V^c_{H,h}$ with

$$\int_\Omega A\nabla\psi^{H,c}_{e^{\cdot}_{II}} \cdot \nabla v^c_H + b\psi^{H,c}_{e^{\cdot}_{II}} v^c_H \, dx = \int_\Omega g(\psi^h_{e^{\cdot}_{II}}, e^c_H, u) v^c_H \, dx$$

for all $v^c_H \in V^c_{H,h}$. Since equally $\psi^h_{e^{\cdot}_{II}} \in V_h$ fulfills

$$\int_\Omega A\nabla\psi^h_{e^{\cdot}_{II}} \cdot \nabla v_h + b\psi^h_{e^{\cdot}_{II}} v_h \, dx = \int_\Omega g(\psi^h_{e^{\cdot}_{II}}, e^c_H, u) v_h \, dx$$

for all $v_h \in V_h$, we obtain by using the $a(\cdot, \cdot)$-orthogonality of $\psi^h_{e^{\cdot}_{II}}$ and $\psi^{H,c}_{e^c_H}$

$$\begin{aligned}
a(\psi^h_{e^{\cdot}_{II}} - \psi^{H,c}_{e^{\cdot}_{II}}, \psi^h_{e^{\cdot}_{II}} - \psi^{H,c}_{e^{\cdot}_{II}}) &= \int_\Omega g(\psi^h_{e^{\cdot}_{II}}, e^c_H, u)(\psi^h_{e^{\cdot}_{II}} - \psi^{H,c}_{e^c_H}) \, dx \\
&\leq \int_\Omega g(\psi^h_{e^{\cdot}_{II}}, e^c_H, u)(\mathrm{Id} - I_H)(\psi^h_{e^{\cdot}_{II}} - \psi^{H,c}_{e^{\cdot}_{II}}) \, dx \\
&\lesssim (\lambda\|\psi^h_{e^{\cdot}_{II}}\|_{H^1(\Omega)} + \|e^c_H\|_{L^2(\Omega)})H\|\nabla(\psi^h_{e^{\cdot}_{II}} - \psi^{H,c}_{e^c_H})\|_{L^2(\Omega)}.
\end{aligned}$$

Since

$$\|\psi^h_{e^{\cdot}_{II}}\|^2_{H^1(\Omega)} \lesssim c_{\lambda,u}(\psi^h_{e^{\cdot}_{II}}, \psi^h_{e^{\cdot}_{II}}) = (e^c_H, \psi^h_{e^{\cdot}_{II}})_{L^2(\Omega)},$$

we get

$$\|\psi^h_{e^{\cdot}_{II}} - \psi^{H,c}_{e^{\cdot}_{II}}\|_{H^1(\Omega)} \lesssim H(\|e^c_H\|_{L^2(\Omega)} + \lambda\|\psi^h_{e^{\cdot}_{II}}\|_{H^1(\Omega)}) \lesssim (1+\lambda)H\|e^c_H\|_{L^2(\Omega)}.$$

Combining this estimate with (6.22) yields

$$\begin{aligned}
\|u - u^c_H\|_{L^2(\Omega)} &\lesssim \left(\frac{\|\psi_{u-u^{\cdot}_{II}} - \psi^h_{e^{\cdot}_{II}}\|_{H^1(\Omega)}}{\|u - u^c_H\|_{L^2(\Omega)}} + \frac{\|\psi^h_{e^{\cdot}_{II}} - \psi^{H,c}_{e^{\cdot}_{II}}\|_{H^1(\Omega)}}{\|u - u^c_H\|_{L^2(\Omega)}}\right) \|u - u^c_H\|_{H^1(\Omega)} \\
&\lesssim \left(\frac{\|\psi_{u-u^{\cdot}_{II}} - \psi^h_{e^{\cdot}_{II}}\|_{H^1(\Omega)}}{\|u - u^c_H\|_{L^2(\Omega)}} + (1+\lambda)H\right) \|u - u^c_H\|_{H^1(\Omega)} \\
&\lesssim \left(\min_{\psi^h \in V_h} \frac{\|\psi_{u-u^{\cdot}_{II}} - \psi^h\|_{H^1(\Omega)}}{\|u - u^c_H\|_{L^2(\Omega)}} + H\right) \|u - u^c_H\|_{H^1(\Omega)}.
\end{aligned}$$

In the last step we used Céa's lemma for linear elliptic problems and the fact that the H^1-best-approximation in the orthogonal space $V^\perp_u \cap V_h$ can be bounded by the H^1-best-approximation in the full space V_h (cf. [13] and equation (40) therein).   □

Using (4.1) and Lemma 6.7 we obtain for $e_H^c := u - u_H^c$

$$\|e_H^c\|_{L^2(\Omega)} \lesssim \left(\min_{\psi^h \in V_h} \frac{\|\psi_{u-u_H^c} - \psi^h\|_{H^1(\Omega)}}{\|e_H^c\|_{L^2(\Omega)}} + H \right) \|e_H^c\|_{H^1(\Omega)} \lesssim (|e_h^0| + H)(|e_h^1| + H^2),$$

where $|e_h^1| := \min_{v_h \in V_h} \|u - v_h\|_{H^1(\Omega)}$ and $|e_h^0| := \min_{\psi^h \in V_h} \frac{\|\psi_{u-u_H^c} - \psi^h\|_{H^1(\Omega)}}{\|u-u_H^c\|_{L^2(\Omega)}}$. Together with (6.19) this yields

$$\begin{aligned}|\lambda - \lambda_H^c| &\lesssim \|e_H^c\|_{H^1(\Omega)}^2 + \|e_H^c\|_{L^2(\Omega)} \\ &\lesssim (|e_h^1| + H^2)^2 + (|e_h^0| + H)(|e_h^1| + H^2) \lesssim H|e_h^1| + H^3.\end{aligned}$$

6.4. Proof of Theorem 4.2. Again, we split the proof into two subsections, one concerning the H^1-error estimate and the other the L^2-error estimate.

6.4.1. Proof of the H^1-error estimate (4.3). Due to the definitions of u_h and u_h^c we get for $v_h \in V_h$

$$\begin{aligned}a(u_h - u_h^c, v_h) &= \lambda_h(u_h, v_h) - \lambda_H^c(u_H^c, v_h) - \beta(|u_h|^2 u_h, v_h)_{L^2(\Omega)} + \beta(|u_H^c|^2 u_H^c, v_h)_{L^2(\Omega)} \\ &= \lambda_h(u_h - u_H^c, v_h) + (\lambda_h - \lambda_H^c)(u_H^c, v_h) \\ &\quad - \beta \sum_{i=0}^2 ((u_h)^{2-i}(u_H^c)^i(u_h - u_H^c), v_h)_{L^2(\Omega)}.\end{aligned}$$

The treatment of the first and the second term in this error identity is obvious. The last term is treated with the Hölder inequality and the embedding $H_0^1(\Omega) \hookrightarrow L^6(\Omega)$ (for $d \le 3$):

$$\begin{aligned}\sum_{i=0}^2 &((u_h)^{2-i}(u_H^c)^i(u_h - u_H^c), v_h)_{L^2(\Omega)} \\ &\le \|u_h\|_{L^6(\Omega)}^2 \|u_h - u_H^c\|_{L^2(\Omega)} \|v_h\|_{L^6(\Omega)} \\ &\quad + \|u_h\|_{L^6(\Omega)} \|u_H^c\|_{L^6(\Omega)} \|u_h - u_H^c\|_{L^2(\Omega)} \|v_h\|_{L^6(\Omega)} \\ &\quad + \|u_H^c\|_{L^6(\Omega)}^2 \|u_h - u_H^c\|_{L^2(\Omega)} \|v_h\|_{L^6(\Omega)} \\ &\lesssim \|u_h\|_{H^1(\Omega)}^2 \|u_h - u_H^c\|_{L^2(\Omega)} \|v_h\|_{H^1(\Omega)} \\ &\quad + \|u_h\|_{H^1(\Omega)} \|u_H^c\|_{H^1(\Omega)} \|u_h - u_H^c\|_{L^2(\Omega)} \|v_h\|_{H^1(\Omega)} \\ &\quad + \|u_H^c\|_{H^1(\Omega)}^2 \|u_h - u_H^c\|_{L^2(\Omega)} \|v_h\|_{H^1(\Omega)}.\end{aligned}$$

We therefore get with $v_h = u_h - u_h^c$ and the Poincaré–Friedrichs inequality

$$\|u_h - u_h^c\|_{H^1(\Omega)} \lesssim (\lambda_h + \lambda_H^c)\|u_h - u_H^c\|_{L^2(\Omega)} + |\lambda_h - \lambda_H^c|.$$

This implies (4.3).

6.4.2. Proof of the L^2-error estimate in (4.4). We start with a lemma that allows us to formulate an error identity.

LEMMA 6.8. *Let $v \in H_0^1(\Omega)$ be an arbitrary function with $\|v\|_{L^2(\Omega)} = 1$ and let $\psi_{u-v} \in V_u^\perp$ denote the corresponding solution of the adjoint problem with*

$$c_{\lambda,u}(\psi_{u-v}, w_\perp) = (u - v, w_\perp)_{L^2(\Omega)}$$

for all $w_\perp \in V_u^\perp$ (cf. (6.18)). Then it holds that

$$\|u - v\|_{L^2(\Omega)}^2 = c_{\lambda,u}(v - u, \psi_{u-v}) + \|u - v\|_{L^2(\Omega)}^2 \int_\Omega |u|^2 u \psi_{u-v}\, dx + \frac{1}{4}\|u - v\|_{L^2(\Omega)}^4.$$

The lemma can be extracted from the proofs given in [13, pp. 99–100].

The following lemma treats the semidiscrete case, i.e., we assume $V_h = H_0^1(\Omega)$. The reason is that the proof of the fully discrete case becomes very technical and hard to read. We note that the proof of the semidiscrete case analogously transfers to the fully discrete case with sufficiently small h by inserting additional continuous approximations to overcome the problems produced by the missing uniform bounds for $\|u_h\|_{L^\times(\Omega)}$ and $\|u_h^c\|_{L^\times(\Omega)}$. For the reader's convenience we therefore only prove the case $h = 0$.

LEMMA 6.9 (estimate (4.4) for $h = 0$). *Assume $h = 0$, i.e., $V_h = H_0^1(\Omega)$. Accordingly we let $u_0^c \in H_0^1(\Omega)$ denote the semidiscrete postprocessed approximation, i.e., the solution to the problem*

$$\int_\Omega A\nabla u_0^c \cdot \nabla\phi\, dx + \int_\Omega b u_0^c \phi\, dx = \lambda_H^c \int_\Omega u_H^c \phi\, dx - \int_\Omega \beta |u_H^c|^2 u_H^c \phi\, dx$$

for all $\phi \in H_0^1(\Omega)$ (cf. Problem 3.5). Then it holds that

$$\|u - u_0^c\|_{L^2(\Omega)} \lesssim H^4.$$

Proof. We divide the proof into two steps. We want to make use of the error identity in Lemma 6.8 with $v = u_0^c$. However, u_0^c is not L^2-normalized and therefore no admissible test function in the error identity. In the first step, we therefore show that the normalization only produces an error of order H^4. In the second step it remains to show that the L^2-error between u and the L^2-normalized u_0^c is also of order H^4.

Step 1. We show that $\left| \|u_H^c\|_{L^2(\Omega)} - \|u_0^c\|_{L^2(\Omega)} \right| \lesssim H^4$, which implies $1 - H^4 \lesssim \|u_0^c\|_{L^2(\Omega)} \lesssim 1 + H^4$ (because of $\|u_H^c\|_{L^2(\Omega)} = 1$).

First observe that $u_0^c \in H_0^1(\Omega)$ is the solution to a classical elliptic problem, which is why we obtain

(6.23) $$\|u_0^c\|_{L^\times} \lesssim \lambda_H^c \lesssim \lambda.$$

Since $a(u_0^c - u_H^c, v_H^c) = 0$ for all $v_H^c \in V_{H,0}^c$ we get $u_0^c - u_H^c \in V_{H,0}^f$. Hence

$$\begin{aligned}
a(u_0^c - u_H^c, u_0^c - u_H^c) &= a(u_0^c, u_0^c - u_H^c) \\
&= \lambda_H^c(u_H^c, u_0^c - u_H^c) - \beta(|u_H^c|^2 u_H^c, u_0^c - u_H^c) \\
&= \lambda_H^c(u_H^c, u_0^c - u_H^c) - \beta(|u_H^c|^2 u_H^c - |u|^2 u, u_0^c - u_H^c) \\
&\quad - \beta(|u|^2 u, u_0^c - u_H^c).
\end{aligned}$$

Using $u_0^c - u_H^c \in V_{H,0}^f$ and inserting $I_H(u_H^c)$ and $I_H(u)$ several times, we get with similar arguments as above and with the previous estimate for $u_H^c - u$

$$\|u_0^c - u_H^c\|_{H^1(\Omega)} \lesssim H^2$$

and

(6.24)

$$\|u_0^c - u_H^c\|_{L^2(\Omega)} = \|(u_0^c - u_H^c) - I_H(u_0^c - u_H^c)\|_{L^2(\Omega)} \lesssim H\|u_0^c - u_H^c\|_{H^1(\Omega)} \lesssim H^3.$$

Next, we show that $\left| \|u_0^c\|_{L^2(\Omega)} - 1 \right|$ is of higher order. We start with

$$
\begin{aligned}
\|u_0^c\|_{H^1(\Omega)}^2 - \|u_H^c\|_{H^1(\Omega)}^2 &= a(u_0^c, u_0^c) - a(u_H^c, u_H^c) \\
&= \lambda_H^c(u_H^c, u_0^c - u_H^c)_{L^2(\Omega)} - \beta(|u_H^c|^2 u_H^c, (u_0^c - u_H^c))_{L^2(\Omega)} \\
&= \lambda_H^c(u_H^c - I_H(u_H^c), u_0^c - u_H^c)_{L^2(\Omega)} \\
&\quad - \beta(|u_H^c|^2 u_H^c - |u_0^c|^2 u_0^c, (u_0^c - u_H^c))_{L^2(\Omega)} - \beta(|u_0^c|^2 u_0^c, (u_0^c - u_H^c))_{L^2(\Omega)} \\
&\stackrel{(6.24)}{\lesssim} (H^4 + H^6 - \beta(|u_0^c|^2 u_0^c, u_0^c - u_H^c)_{L^2(\Omega)}.
\end{aligned}
$$

Using that u_0^c is bounded uniformly in $L^\infty(\Omega)$ we can proceed as in the proof of Lemma 6.5 to show

$$
\beta(|u_0^c|^2 u_0^c, u_0^c - u_H^c)_{L^2(\Omega)} \lesssim H \|u_0^c\|_{H^1(\Omega)} \|u_0^c - u_H^c\|_{L^2(\Omega)} \lesssim H^4.
$$

So in summary,

$$
\left| \|u_0^c\|_{H^1(\Omega)}^2 - \|u_H^c\|_{H^1(\Omega)}^2 \right| \lesssim H^4.
$$

However, on the other hand,

$$
\begin{aligned}
\lambda_H^c\left(\|u_H^c\|_{L^2(\Omega)}^2 - \|u_0^c\|_{L^2(\Omega)}^2 \right) &= \lambda_H^c(u_H^c - u_0^c, u_0^c - I_H(u_0^c))_{L^2(\Omega)} \\
&\quad - \beta(|u_H^c|^2 u_H^c, (u_0^c - u_H^c))_{L^2(\Omega)} \\
&\quad - \|u_0^c\|_{H^1(\Omega)}^2 + \|u_H^c\|_{H^1(\Omega)}^2.
\end{aligned}
$$

This we can treat with the previous results to get

$$
\left| \|u_H^c\|_{L^2(\Omega)}^2 - \|u_0^c\|_{L^2(\Omega)}^2 \right| \lesssim H^4.
$$

With $\|u_H^c\|_{L^2(\Omega)} = 1$ we get

$$
(6.25) \qquad \left| \|u_H^c\|_{L^2(\Omega)} - \|u_0^c\|_{L^2(\Omega)} \right| \leq \left| \|u_H^c\|_{L^2(\Omega)}^2 - \|u_0^c\|_{L^2(\Omega)}^2 \right| \lesssim H^4.
$$

Note that in the last step we used that for any $a \geq 0$ it holds that $|1 - a| \leq |1 - a^2|$.

Step 2. Step 1 justifies the definition of $\tilde{u}_0^c := \|u_0^c\|_{L^2(\Omega)}^{-1} u_0^c$ which fulfills

$$
(6.26) \qquad \|\tilde{u}_0^c - u_0^c\|_{L^2(\Omega)} = \left| \|u_0^c\|_{L^2(\Omega)} - 1 \right| \|u_0^c\|_{L^2(\Omega)} \lesssim H^4.
$$

Next, we show $\|u - \tilde{u}_0^c\|_{L^2(\Omega)} \lesssim H^4$. For this purpose define $\bar{\lambda}_H^c := \|u_0^c\|_{L^2(\Omega)}^{-1} \lambda_H^c$. Then $\tilde{u}_0^c \in H_0^1(\Omega)$ solves

$$
\int_\Omega A \nabla \tilde{u}_0^c \cdot \nabla \phi \, dx + \int_\Omega b \tilde{u}_0^c \phi \, dx = \bar{\lambda}_H^c \int_\Omega u_H^c \phi \, dx - \int_\Omega \frac{\beta}{\|u_0^c\|_{L^2(\Omega)}} |u_H^c|^2 u_H^c \phi \, dx.
$$

We want to use Lemma 6.8 and denote $\psi := \psi_{u-\tilde{u}_0^c}$ with $\psi_{u-\tilde{u}_0^c} \in V_u^{\perp}$ being the solution of (6.18) for $w = u - \tilde{u}_0^c$. Before we start to estimate $c_{\lambda,u}(\tilde{u}_0^c - u, \psi)$ observe that $(u, \psi)_{L^2(\Omega)} = 0$ (by definition), which yields

$$
\begin{aligned}
(6.27) \qquad \lambda_H^c(u_H^c, \psi)_{L^2(\Omega)} - \lambda(\tilde{u}_0^c, \psi)_{L^2(\Omega)} &= (\lambda_H^c - \lambda)(u_H^c - u, \psi)_{L^2(\Omega)} \\
&\quad + \lambda(u_H^c - u_0^c, \psi)_{L^2(\Omega)} + \lambda(u_0^c - \tilde{u}_0^c, \psi)_{L^2(\Omega)}.
\end{aligned}
$$

We get

$$
\begin{aligned}
c_{\lambda,u}&(\tilde{u}_0^c - u, \psi) \\
&= a(\tilde{u}_0^c - u, \psi) + 3\beta \int_\Omega |u|^2 \tilde{u}_0^c \psi \, dx - 3\beta \int_\Omega |u|^2 u \psi \, dx - \lambda(\tilde{u}_0^c, \psi)_{L^2(\Omega)} + \lambda(u, \psi)_{L^2(\Omega)} \\
&= a(\tilde{u}_0^c, \psi) + 3\beta \int_\Omega |u|^2 \tilde{u}_0^c \psi \, dx - 2\beta \int_\Omega |u|^2 u \psi \, dx - \lambda(\tilde{u}_0^c, \psi)_{L^2(\Omega)} \\
&= \left(\frac{1 - \|u_0^c\|_{L^2(\Omega)}}{\|u_0^c\|_{L^2(\Omega)}} + 1 \right) \left(\lambda_H^c \int_\Omega u_H^c \psi \, dx - \beta \int_\Omega |u_H^c|^2 u_H^c \psi \, dx \right) \\
&\quad + 3\beta \int_\Omega |u|^2 \tilde{u}_0^c \psi \, dx - 2\beta \int_\Omega |u|^2 u \psi \, dx - \lambda(\tilde{u}_0^c, \psi)_{L^2(\Omega)} \\
&\stackrel{(6.27)}{=} \underbrace{\left(\frac{1 - \|u_0^c\|_{L^2(\Omega)}}{\|u_0^c\|_{L^2(\Omega)}} \right) (\lambda_H^c u_H^c - \beta|u_H^c|^2 u_H^c, \psi)_{L^2(\Omega)}}_{=:I} + \underbrace{(\lambda_H^c - \lambda)(u_H^c - u, \psi)_{L^2(\Omega)}}_{=:II} \\
&\quad + \underbrace{\lambda(u_H^c - u_0^c, \psi - I_H(\psi))_{L^2(\Omega)}}_{=:III} + \underbrace{\lambda(u_0^c - \tilde{u}_0^c, \psi)_{L^2(\Omega)}}_{=:IV} \\
&\quad + \underbrace{3\beta(|u|^2(\tilde{u}_0^c - u_0^c), \psi)_{L^2(\Omega)}}_{=:V} + \underbrace{3\beta(|u|^2(u_0^c - u_H^c), \psi)_{L^2(\Omega)}}_{=:VI} \\
&\quad - \underbrace{\beta \int_\Omega (u - u_H^c)^2(u_H^c + 2u)\psi \, dx}_{=:VII}.
\end{aligned}
$$

In the last step we used $(u, \psi)_{L^2(\Omega)} = 0$ and

$$
a^3 - 3ab^2 + 2b^3 = (a - b)^2(a + 2b) \quad \text{for } a, b \in \mathbb{R}.
$$

With (6.25) we have

$$
|I| \lesssim \left| \frac{1 - \|u_0^c\|_{L^2(\Omega)}}{\|u_0^c\|_{L^2(\Omega)}} \right| (\lambda_H^c + \|u_H^c\|_{H^1(\Omega)}^3)\|\psi\|_{L^2(\Omega)} \lesssim H^4 \lambda_H^c (1 + (\lambda_H^c)^2)\|\psi\|_{H^1(\Omega)}.
$$

For II we use Theorem 4.1 to obtain

$$
|II| \leq |\lambda_H^c - \lambda|\|u_H^c - u\|_{L^2(\Omega)}\|\psi\|_{L^2(\Omega)} \lesssim H^3 H^3 \|\psi\|_{L^2(\Omega)} \leq H^6 \|\psi\|_{H^1(\Omega)}.
$$

For term III we can use (6.24), which gives us

$$
|III| \leq \lambda|(u_H^c - u_0^c, \psi - I_H(\psi))_{L^2(\Omega)}| \lesssim \lambda H^3 \|\psi - I_H(\psi)\|_{L^2(\Omega)} \lesssim H^4 \|\psi\|_{H^1(\Omega)}.
$$

Using (6.26) we get

$$|\mathrm{IV}| \leq \lambda \|u_0^c - \bar{u}_0^c\|_{L^2(\Omega)} \|\psi\|_{L^2(\Omega)} \lesssim H^4 \|\psi\|_{H^1(\Omega)}.$$

Equally we get

$$|\mathrm{V}| \lesssim |(|u|^2(\bar{u}_0^c - u_0^c), \psi)_{L^2(\Omega)}| \lesssim \|u\|_{L^6(\Omega)}^2 \|\bar{u}_0^c - u_0^c\|_{L^2(\Omega)} \|\psi\|_{L^6(\Omega)} \lesssim \lambda H^4 \|\psi\|_{H^1(\Omega)}.$$

To estimate VI we need the L^∞-estimate given by (6.21), which reads

$$(6.28) \qquad \|\psi_{u-\tilde{u}_0^c}\|_{L^\infty(\Omega)} \lesssim \|\bar{u}_0^c - u\|_{L^2(\Omega)}.$$

For $z \in \mathcal{N}_H$, let the values u_z and ψ_z denote the coefficients appearing in the weighted Clément interpolation of u and ψ (cf. (3.2)). Recall that Φ_z denote the nodal basis functions of V_H. Using again (6.24), $(\Phi_z, u^f)_{L^2(\Omega)} = 0$ for all $z \in \mathcal{N}_H$, and the fact that $u_0^c - u_H^c \in V_{H,0}^f$, we obtain

$$\begin{aligned}
|\mathrm{VI}| &\lesssim |(|u|^2(u_0^c - u_H^c), \psi)_{L^2(\Omega)}| \\
&= \left| ((u - I_H(u))u\psi, u_0^c - u_H^c)_{L^2(\Omega)} + \sum_{z \in \mathcal{N}_H} (u_z(u - u_z)\psi\Phi_z, u_0^c - u_H^c)_{L^2(\Omega)} \right. \\
&\quad \left. + \sum_{z \in \mathcal{N}_H} (|u_z|^2(\psi - \psi_z)\Phi_z, u_0^c - u_H^c)_{L^2(\Omega)} \right| \\
&\lesssim \|u\|_{L^\infty(\Omega)} \left(2\|\psi\|_{L^\infty(\Omega)}\|u\|_{H^1(\Omega)} + \|u\|_{L^\infty(\Omega)}\|\psi\|_{H^1(\Omega)} \right) H\|u_0^c - u_H^c\|_{L^2(\Omega)} \\
&\overset{(6.28)}{\lesssim} H^4 \|\tilde{u}_0^c - u\|_{L^2(\Omega)}.
\end{aligned}$$

For the last term Theorem 4.1 leads to

$$|\mathrm{VII}| \lesssim \|u - u_H^c\|_{H^1(\Omega)}^2 \left(\|u_H^c\|_{L^2(\Omega)} + 2\|u\|_{L^2(\Omega)} \right) \|\psi\|_{H^1(\Omega)} \lesssim H^4 \|\psi\|_{H^1(\Omega)}.$$

Combining the results for terms I–VII and using $\|\psi\|_{H^1(\Omega)} \lesssim \|\bar{u}_0^c - u\|_{L^2(\Omega)}$ we get

$$|c_{\lambda,u}(\bar{u}_0^c - u, \psi)| \lesssim H^4 \|\tilde{u}_0^c - u\|_{L^2(\Omega)}.$$

Since (by using the previous estimate for $\|u - \tilde{u}_0^c\|_{H^1(\Omega)}$)

$$\frac{1}{4}\|u - \tilde{u}_0^c\|_{L^2(\Omega)}^4 + \|u - \tilde{u}_0^c\|_{L^2(\Omega)}^2 \int_\Omega |u|^2 u\psi_{u-\tilde{u}_0^c}\, dx \leq CH^3 \|u - \bar{u}_0^c\|_{L^2(\Omega)}^2$$

we finally obtain with Lemma 6.8

$$\|u - \tilde{u}_0^c\|_{L^2(\Omega)}^2 \lesssim |c_{\lambda,u}(\bar{u}_0^c - u, \psi)| \lesssim H^4 \|\bar{u}_0^c - u\|_{L^2(\Omega)}.$$

With (6.24) we therefore proved

$$\|u - u_0^c\|_{L^2(\Omega)} \lesssim H^4. \qquad \square$$

PROPOSITION 6.10. *The L^2-error estimate in the fully discrete case can be proved analogously to the semidiscrete case above. We therefore get for sufficiently small h that*

$$\|u - u_h^c\|_{L^2(\Omega)} \lesssim H^4 + C_{L^2}(h, H)$$

with $C_{L^2}(h, H)$ behaving like the term $H^2\|u - u_h\|_{H^1(\Omega)}$.

6.4.3. Proof of the eigenvalue error estimate in (4.4). From the following corollary we can conclude estimate (4.4).

COROLLARY 6.11. *Let $u_h^c \in V_h$ denote the solution of the postprocessing step defined via Problem 3.5 and let $\lambda_h^c := (2E(u_h^c) + 2^{-1}\beta\|u_h^c\|_{L^4(\Omega)}^4)\|u_h^c\|_{L^2(\Omega)}^{-2}$. Then there holds*

$$|\lambda_h - \lambda_h^c| \lesssim \|u_h - u_h^c\|_{H^1(\Omega)}^2 + \|u_h - u_h^c\|_{L^2(\Omega)}.$$

Proof. We have for arbitrary $v_h \in V_h$

$$a(u_h - v_h, u_h - v_h) + \beta(|u_h|^2(u_h - v_h), u_h - v_h)_{L^2(\Omega)} - \lambda_h(u_h - v_h, u_h - v_h)_{L^2(\Omega)}$$
$$= a(v_h, v_h) - \lambda_h(v_h, v_h) + \beta(|u_h|^2 v_h, v_h)_{L^2(\Omega)}.$$

This implies with $v_h = u_h^c$

$$
|\lambda_h^c - \lambda_h| = \left| \frac{a(u_h^c, u_h^c) + \beta(|u_h^c|^2 u_h^c, u_h^c)_{L^2(\Omega)} - \lambda_h\|u_h^c\|_{L^2(\Omega)}^2}{\|u_h^c\|_{L^2(\Omega)}^2} \right|
$$
$$
= \left| \frac{\|u_h - u_h^c\|_{H^1(\Omega)}^2 + \beta(|u_h|^2, (u_h - u_h^c)^2)_{L^2(\Omega)} - \lambda_h\|u_h - u_h^c\|_{L^2(\Omega)}^2}{\|u_h^c\|_{L^2(\Omega)}^2} \right.
$$
$$
\left. + \frac{\beta((|u_h|^2 - |u_h^c|^2), |u_h^c|^2)_{L^2(\Omega)}}{\|u_h^c\|_{L^2(\Omega)}^2} \right|.
$$

The remaining estimate is straightforward using $(a^2 - b^2) = (a - b)(a + b)$. Note that the last term is the dominating term.   □

We obtain (4.4) from Corollary 6.11 and our previous estimates for $\|u - u_h^c\|_{H^1(\Omega)}$ and $\|u - u_h^c\|_{L^2(\Omega)}$.

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