Mixed finite elements for the Gross–Pitaevskii eigenvalue problem: *a priori* error analysis and guaranteed lower energy bound

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We establish an *a priori* error analysis for the lowest-order Raviart–Thomas finite element discretization of the nonlinear Gross-Pitaevskii eigenvalue problem. Optimal convergence rates are obtained for the primal and dual variables as well as for the eigenvalue and energy approximations. In contrast to conforming approaches, which naturally imply upper energy bounds, the proposed mixed discretization provides a guaranteed and asymptotically exact lower bound for the ground state energy. The theoretical results are illustrated by a series of numerical experiments.

Keywords: Gross–Pitaevskii eigenvalue problem; mixed finite elements; lower bounds; *a priori* error analysis.

1. Introduction

We study the Gross–Pitaevskii equation (GPE), a nonlinear eigenvalue problem that describes the quantum states of bosonic particles at ultracold temperatures, so-called Bose–Einstein condensates. Given a convex Lipschitz domain $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$), the GPE searches for L^2-normalised eigenstates $\{u_j : j \in \mathbb{N}\} \subset H^1_0(\Omega)$ and corresponding eigenvalues $\lambda_j \in \mathbb{R}$ 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. Here, $V \in L^\infty(\Omega)$ denotes a non-negative trapping potential that confines the particles to a particular region within the domain, and κ is a positive constant. Note that all eigenvalues of

(1.1) are real and positive and that the smallest eigenvalue is simple. Assuming a nondecreasing ordering of the eigenvalues, this means that $0 < \lambda_1 < \lambda_2 \leq \dots$.

The nonlinear eigenvalue problem (1.1) is the Euler–Lagrange equation for critical points of the Gross–Pitaevskii energy

$$\mathcal{E}(v) := \frac{1}{2}(\nabla v, \nabla v)_{L^2} + \frac{1}{2}(Vv, v)_{L^2} + \frac{\kappa}{4}(|v|^2 v, v)_{L^2}, \quad v \in H^1_0(\Omega), \tag{1.2}$$

subject to the L^2-normalization constraint. Of particular physical interest is the ground state of the Gross–Pitaevskii energy, characterised by

$$u \in \underset{v \in H^1_0(\Omega)\,:\,\|v\|_{L^2}=1}{\arg\min} \mathcal{E}(v). \tag{1.3}$$

We emphasise that under the above assumptions on Ω and V, the global energy minimiser exists and is unique up to sign. Furthermore, the ground state u (up to sign) coincides with the eigenstate u_1 corresponding to the smallest eigenvalue λ_1 of (1.1). The minimal energy E is related to the smallest eigenvalue λ_1 by $\lambda_1 = 2E + \frac{\kappa}{2}\|u\|^4_{L^4}$. Note that the above theoretical results on the Gross–Pitaevskii problem can be found, e.g., in Cancès *et al.* (2010).

There are a number of discretizations in the literature to approximate the ground state of the GPE. Such discretizations are typically based on H^1_0-conforming methods, such as standard continuous finite elements Zhou (2004); Cancès *et al.* (2010); Chen *et al.* (2011), spectral and pseudospectral methods Cancès *et al.* (2010); Bao & Cai (2013), multiscale methods Henning *et al.* (2014); Henning & Wärnegård (2022); Henning & Persson (2023); Peterseim *et al.* (2024) and mesh-adaptive methods Danaila & Hecht (2010); Heid *et al.* (2021). Very recently, also nonstandard conforming finite element discretizations based on mass lumping with certain positivity preservation properties were proposed in Hauck *et al.* (2024); Chen *et al.* (2024a). Note that standard conforming discretizations have in common that the ground state energy is approximated from above, as the energy is minimised in a subspace. In this work we instead use a mixed finite element discretization, which allows asymptotically exact lower bounds on the ground state energy. In the linear setting such an approach has recently been introduced in Gallistl (2023).

In addition to the guaranteed lower energy bound, we provide a rigorous *a priori* error analysis of the proposed mixed finite element method for the GPE. We prove first-order convergence for the primal and dual variables in the L^2-norm and second-order convergence for the energy and eigenvalue approximations. So far, error estimates of this form have only been shown for conforming approximations of the primal variable. Although there is a large body of work on mixed discretization methods for linear eigenvalue problems (see, e.g., the review article Boffi (2010)), mixed discretizations of nonlinear eigenvector problems have not yet been addressed. In fact, the present error analysis differs substantially from the established techniques used in the linear case and is inspired by existing work Zhou (2004); Cancès *et al.* (2010) for conforming methods.

2. Mixed finite element discretization

Consider a hierarchy of simplicial meshes $\{\mathcal{T}_h\}_{h>0}$ of the domain Ω, which we assume to be geometrically conforming (cf. (Ern & Guermond, 2004, Def. 1.55)) and shape-regular (cf. (Ern & Guermond, 2004, Def. 1.107)). We denote the elements of any mesh $\mathcal{T}_h$ in the hierarchy by K and define the mesh size

h as the maximum diameter of elements in $\mathcal{T}_h$, i.e., $h := \max_{K\in\mathcal{T}_h} \operatorname{diam} K$. For the mixed discretization of the Gross–Pitaevskii problem, we use the finite element pair (Σ_h, U_h), where Σ_h denotes the lowest-order Raviart–Thomas finite element space with respect to $\mathcal{T}_h$ (see, e.g., (Ern & Guermond, 2004, Ch. 1.2.7)) and U_h is the space of $\mathcal{T}_h$-piecewise constants. A discrete analogue of the gradient operator $G_h \colon U_h \to \Sigma_h$ is defined for arbitrary $v_h \in U_h$ by the property

$$(G_h v_h, \tau_h)_{L^2} + (\operatorname{div} \tau_h, v_h)_{L^2} = 0, \tag{2.1}$$

for all $\tau_h \in \Sigma_h$. The discrete gradient gives rise to the discrete energy defined for any $v_h \in U_h$ by

$$\mathcal{E}_h(v_h) := \frac{1}{2}(G_h v_h, G_h v_h)_{L^2} + \frac{1}{2}(V v_h, v_h)_{L^2} + \frac{\kappa}{4}(|v_h|^2 v_h, v_h)_{L^2}.$$

A discrete approximation $u_h \in U_h$ of the ground state u in the Raviart–Thomas space is then obtained as the solution of the finite-dimensional minimization problem

$$u_h \in \operatorname*{arg\,min}_{v_h\in U_h \colon \|v_h\|_{L^2}=1} \mathcal{E}_h(v_h). \tag{2.2}$$

Note that in the discrete setting the boundedness of the norms of the minimising sequence directly implies the strong convergence of a subsequence (Bolzano–Weierstrass theorem). Thus, there always exist discrete energy minimisers u_h and $-u_h$. Unlike in the continuous setting, cf. (1.3), the solution u_h to (2.2) is not unique up to sign in general. To have compatible signs of the ground state and its discrete approximation we choose the sign of u_h such that $(u, u_h)_{L^2} \geq 0$.

The proof of the guaranteed lower energy bound is based on certain properties of the operators $\pi_h \colon L^2(\Omega) \to U_h$ and $\Pi_h \colon (L^2(\Omega))^d \to \Sigma_h$, which are defined as L^2-projections onto U_h and Σ_h, respectively. By definition, π_h and Π_h are bounded with respect to the L^2-norm with constant one. Moreover, for π_h we get by Poincaré's inequality Payne & Weinberger (1960) that, for all $K \in \mathcal{T}_h$ and for all $v \in H^1(K)$,

$$\|v - \pi_h v\|_{L^2(K)} \leq \pi^{-1} h \|\nabla v\|_{L^2(K)}, \tag{2.3}$$

where we write $L^2(K)$ for the restriction of the L^2-space and its associated inner product and norm to the element K. If no subdomain is specified, we always refer to the L^2-space on the whole domain. The following lemma from Gallistl (2023) establishes a crucial commuting property for the operators π_h and Π_h.

Lemma 2.1. (Commuting property) Any $v \in H^1_0(\Omega)$ satisfies $G_h \pi_h v = \Pi_h \nabla v$.

Proof. Using (2.1) and integration by parts we obtain that

$$(G_h \pi_h v, \tau_h)_{L^2} = -(\operatorname{div} \tau_h, \pi_h v)_{L^2} = -(\operatorname{div} \tau_h, v)_{L^2} = (\nabla v, \tau_h)_{L^2} = (\Pi_h \nabla v, \tau_h)_{L^2}$$

for any $v \in H^1_0(\Omega)$ and $\tau_h \in \Sigma_h$, which is the assertion. $\square$

3. Guaranteed lower energy bound

The following theorem gives a lower bound on the ground state energy $E := \mathcal{E}(u)$ using a modified version of the discrete ground state energy $E_h := \mathcal{E}_h(u_h)$. This is the first major result of this paper.

THEOREM 3.1. (Lower bound) If the potential V is $\mathcal{T}_h$-piecewise constant it holds that

$$E_h^{\mathrm{mod}} := \frac{E_h}{1 + 4h^2\pi^{-2}E_h} \leq E. \tag{3.1}$$

Proof. The discrete energy of the ground state is characterised by the following pseudo-Rayleigh quotient:

$$E_h = \min_{v_h \in U_h \setminus \{0\}} \frac{\frac{1}{2}\|G_h v_h\|_{L^2}^2 \|v_h\|_{L^2}^2 + \frac{1}{2}\|V^{1/2} v_h\|_{L^2}^2 \|v_h\|_{L^2}^2 + \frac{\kappa}{4}\|v_h\|_{L^4}^4}{\|v_h\|_{L^2}^4}.$$

We majorise E_h by choosing $v_h := \pi_h u$. This results in

$$E_h \|v_h\|_{L^2}^4 \leq \frac{1}{2}\|G_h v_h\|_{L^2}^2 \|v_h\|_{L^2}^2 + \frac{1}{2}\|V^{1/2} v_h\|_{L^2}^2 \|v_h\|_{L^2}^2 + \frac{\kappa}{4}\|v_h\|_{L^4}^4. \tag{3.2}$$

We bound all the terms on the right-hand side individually. Using the L^2-stability of π_h we get that

$$\|v_h\|_{L^2}^2 = \|\pi_h u\|_{L^2}^2 \leq \|u\|_{L^2}^2.$$

Since V is assumed to be $\mathcal{T}_h$-piecewise constant we obtain that

$$\|V^{1/2} v_h\|_{L^2}^2 = \|V^{1/2} \pi_h u\|_{L^2}^2 = \sum_{K \in \mathcal{T}_h} V|_K \left\| \fint_K u \,\mathrm{d}x \right\|_{L^2(K)}^2 \leq \|V^{1/2} u\|_{L^2}^2.$$

Lemma 2.1 and the L^2-stability of Π_h yield that

$$\|G_h v_h\|_{L^2}^2 = \|\Pi_h \nabla u\|_{L^2}^2 \leq \|\nabla u\|_{L^2}^2.$$

Finally, the L^4-term is bounded by Jensen's inequality

$$\|v_h\|_{L^4}^4 = \sum_{K \in \mathcal{T}_h} \int_K \left(\quad_K u \,\mathrm{d}x \right)^4 \mathrm{d}x \leq \sum_{K \in \mathcal{T}_h} \int_K \quad_K |u|^4 \,\mathrm{d}x \,\mathrm{d}x = \|u\|_{L^4}^4.$$

Altogether, by inserting the above bounds into (3.2) and using that $\|u\|_{L^2} = 1$ we get that

$$E_h \|v_h\|_{L^2}^4 \leq E.$$

For rewriting the left-hand side we use the Pythagorean identity, which yields that

$$\|v_h\|_{L^2}^4 = \big(\|\pi_h u\|_{L^2}^2\big)^2 = \big(1 - \|u - \pi_h u\|_{L^2}^2\big)^2.$$

Using (2.3) we then obtain the lower bound

$$\|v_h\|_{L^2}^4 \geq \big(1 - h^2\pi^{-2}\|\nabla u\|_{L^2}^2\big)^2 \geq \big(1 - 2h^2\pi^{-2}E\big)^2,$$

where we have used that $\frac{1}{2}\|\nabla u\|_{L^2}^2 \leq E$. The combination of the previous estimates leads to the inequality

$$E_h\big(1 - 2h^2\pi^{-2}E\big)^2 \leq E.$$

Expanding the squared brackets and estimating yields

$$\big(1 - 2h^2\pi^{-2}E\big)^2 = 1 - 4h^2\pi^{-2}E + 4h^4\pi^{-4}E^2 \geq 1 - 4h^2\pi^{-2}E,$$

which implies that

$$E_h\big(1 - 4h^2\pi^{-2}E\big) \leq E. \tag{3.3}$$

Elementary algebra then gives the assertion. □

4. *A priori* error analysis

In this section we perform an *a priori* error analysis of the proposed mixed finite element discretization. We will follow an approach inspired by the analysis of conforming methods, cf. Zhou (2004); Cancès *et al.* (2010). However, the main obstacle is that the mixed formulation is not symmetric positive definite. To overcome this problem, we employ a conforming lifting (see Lemma A.1) and tools from mixed finite element theory to establish a link to conforming methods.

In mixed form, the Gross–Pitaevskii eigenvalue problem for the ground state seeks the pair $(u,\sigma) \in L^2(\Omega) \times H(\operatorname{div},\Omega)$ with $\|u\|_{L^2} = 1$ corresponding to the smallest eigenvalue $\lambda \in \mathbb{R}$ such that

$$(\sigma,\tau)_{L^2} + (\operatorname{div}\tau, u)_{L^2} = 0 \qquad \text{for all } \tau \in H(\operatorname{div},\Omega), \tag{4.1a}$$

$$(\operatorname{div}\sigma, v)_{L^2} - ((\kappa|u|^2 + V)u, v)_{L^2} = -\lambda(u,v)_{L^2} \qquad \text{for all } v \in L^2(\Omega). \tag{4.1b}$$

Similarly, also any discrete ground state $u_h \in U_h$ satisfies a mixed variational eigenvalue problem. More precisely, there exist $\sigma_h = G_h u_h \in \Sigma_h$ and an eigenvalue $\lambda_h \in \mathbb{R}$ such that

$$(\sigma_h,\tau_h)_{L^2} + (\operatorname{div}\tau_h, u_h)_{L^2} = 0 \qquad \text{for all } \tau_h \in \Sigma_h, \tag{4.2a}$$

$$(\operatorname{div}\sigma_h, v_h)_{L^2} - ((\kappa|u_h|^2 + V)u_h, v_h)_{L^2} = -\lambda_h(u_h,v_h)_{L^2} \qquad \text{for all } v_h \in U_h. \tag{4.2b}$$

Note that λ_h may not be the smallest discrete eigenvalue. Similarly as in the continuous setting the discrete energy and discrete ground state eigenvalue are related by $\lambda_h = 2E_h + \frac{\kappa}{2}\|u_h\|_{L^4}^4$.

The error analysis is based on the following elementary identity for the difference of the energies.

LEMMA 4.1. (Energy error characterization) It holds that

$$
\begin{aligned}
E_h - E = &- \frac{1}{2}\|G_h u_h - \nabla u\|_{L^2}^2 - \frac{1}{2}\|V^{1/2}(u_h - u)\|_{L^2}^2 \\
&+ \frac{1}{2}\lambda_h \|u_h - u\|_{L^2}^2 - \frac{\kappa}{4}((u_h - u)^2, 3u_h^2 + 2uu_h + u^2)_{L^2} \\
&+ ((V - \pi_h V)(u_h - u), u_h)_{L^2}.
\end{aligned}
$$

Proof. The definitions of E_h and E together with elementary algebraic manipulations yield that

$$
E_h - E = -\frac{1}{2}\|G_h u_h - \nabla u\|_{L^2}^2 - \frac{1}{2}\|V^{1/2}(u_h - u)\|_{L^2}^2 + R
$$

with

$$
R := (G_h u_h - \nabla u, G_h u_h)_{L^2} + (V(u_h - u), u_h)_{L^2} + \frac{\kappa}{4}(\|u_h\|_{L^4}^4 - \|u\|_{L^4}^4).
$$

From the properties of the L^2-projections π_h and Π_h the identity $\Pi_h \nabla u = G_h \pi_h u$ from Lemma 2.1, and (4.2), we get that

$$
\begin{aligned}
R = &(G_h u_h - \Pi_h \nabla u, G_h u_h)_{L^2} + (\pi_h V(u_h - \pi_h u), u_h)_{L^2} \\
&+ ((V - \pi_h V)(u_h - u), u_h)_{L^2} + \frac{\kappa}{4}(\|u_h\|_{L^4}^4 - \|u\|_{L^4}^4) \\
= &- \kappa(u_h^3, u_h - u)_{L^2} + \lambda_h(u_h, u_h - u)_{L^2} \\
&+ ((V - \pi_h V)(u_h - u), u_h)_{L^2} + \frac{\kappa}{4}(\|u_h\|_{L^4}^4 - \|u\|_{L^4}^4).
\end{aligned}
$$

Since u_h and u are L^2-normalised, we have $\lambda_h(u_h, u_h - u)_{L^2} = \frac{1}{2}\lambda_h\|u_h - u\|_{L^2}^2$. Rearranging the terms and using that

$$
- \kappa(u_h^3, u_h - u)_{L^2} + \frac{\kappa}{4}(\|u_h\|_{L^4}^4 - \|u\|_{L^4}^4) = -\frac{\kappa}{4}((u_h - u)^2, 3u_h^2 + 2uu_h + u^2)_{L^2}
$$

readily yields the assertion. □

REMARK 4.2. (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 and on the ground state u, but is independent of the mesh size h.

The following theorem states a convergence result for the mixed finite element approximation to the ground state.

THEOREM 4.3. (Plain convergence of mixed method) As $h \to 0$ it holds that

$$\|u - u_h\|_{L^2} \to 0, \quad \|G_h u_h - \nabla u\|_{L^2} \to 0, \quad E_h \to E, \quad \lambda_h \to \lambda.$$

Proof. We consider

$$u_h^* \in \operatorname*{arg\,min}_{v \in H_0^1(\Omega)\,:\,\|v\|_{L^2}=1} \mathcal{E}_h^*(v) \tag{4.3}$$

with the modified energy

$$\mathcal{E}_h^*(v) := \frac{1}{2}(\nabla v, \nabla v)_{L^2} + \frac{1}{2}(\pi_h V v, v)_{L^2} + \frac{\kappa}{4}(|v|^2 v, v)_{L^2}, \quad v \in H_0^1(\Omega).$$

Similar as for the Gross–Pitaevskii energy minimization problem (1.3) the global modified energy minimiser exists and is unique up to sign. Note that despite the use of h in the notation (4.3) is a continuous problem. To get the uniqueness of (4.3) we choose the sign of u_h^* such that $(u, u_h^*)_{L^2} \geq 0$ holds. The energies $E_h^* := \mathcal{E}_h^*(u_h^*)$ are uniformly bounded with respect to h since

$$E_h^* \leq \mathcal{E}_h^*(u) = E + \frac{1}{2}((\pi_h V - V)u, u)_{L^2} \lesssim 1 + \|V - \pi_h V\|_{L^2} \lesssim 1,$$

where we used that $E_h^* \leq \mathcal{E}_h^*(u)$ and the L^4-regularity of u. The uniform boundedness of E_h^* directly implies that $\|u_h^*\|_{L^4}$ is uniformly bounded. Using this, we obtain similarly as before the estimates

$$\begin{aligned} |E_h^* - \mathcal{E}(u_h^*)| &= \frac{1}{2}|((\pi_h V - V)u_h^*, u_h^*)_{L^2}| \lesssim \|V - \pi_h V\|_{L^2} \to 0, \\ |\mathcal{E}_h^*(u) - E| &= \frac{1}{2}|((\pi_h V - V)u, u)_{L^2}| \lesssim \|V - \pi_h V\|_{L^2} \to 0. \end{aligned} \tag{4.4}$$

Together with $E \leq \mathcal{E}(u_h^*)$ and $E_h^* \leq \mathcal{E}_h^*(u)$, they imply that

$$\begin{aligned} 0 \leq \mathcal{E}(u_h^*) - E &= \mathcal{E}(u_h^*) - E_h^* + E_h^* - \mathcal{E}_h^*(u) + \mathcal{E}_h^*(u) - E \\ &\leq |E_h^* - \mathcal{E}(u_h^*)| + |\mathcal{E}_h^*(u) - E| \to 0. \end{aligned} \tag{4.5}$$

Combining (4.4) and (4.5) we get that

$$|E - E_h^*| \leq |E_h^* - \mathcal{E}(u_h^*)| + |\mathcal{E}(u_h^*) - E| \to 0. \tag{4.6}$$

Note that the discrete ground state can be interpreted as a discretization of (4.3). This allows us to conclude, similarly to (3.3) in the proof of Theorem 3.1, that

$$E_h\big(1 - 4h^2\pi^{-2}E_h^*\big) \leq E_h^*, \tag{4.7}$$

which implies the uniform boundedness of the discrete energies. As a consequence $\|G_h u_h\|_{L^2}$, $\|u_h\|_{L^4}$ and λ_h are uniformly bounded. Furthermore, by the discrete embedding of Lemma A.4 $\|u_h\|_{L^6}$ is also uniformly bounded.

Using the uniform bounds from above we have that

$$\|\operatorname{div} G_h u_h\|_{L^2} = \|\pi_h(\kappa|u_h|^2 u_h + V u_h - \lambda_h u_h)\|_{L^2} \lesssim 1.$$

This estimate has two consequences: First, by Lemma A.2 it implies the uniform boundedness of $\|u_h\|_{L^\infty}$. Second, denoting by $\tilde{u}_h^c \in H^2(\Omega) \cap H_0^1(\Omega)$ the conforming lifting of u_h from Lemma A.1, we have that

$$\|G_h u_h - \nabla \tilde{u}_h^c\|_{L^2} + \|u_h - \tilde{u}_h^c\|_{L^2} \lesssim h \|\operatorname{div} G_h u_h\|_{L^2} \lesssim h, \tag{4.8}$$

where we used the bound from Lemma A.1. In the following, we consider the L^2-normalised version $u_h^c := \tilde{u}_h^c / \|\tilde{u}_h^c\|_{L^2}$. Using elementary algebra and that $\|u_h\|_{L^2} = 1$ one can show for the normalization constant that

$$\big|\|\tilde{u}_h^c\|_{L^2} - 1\big| = \big|\|\tilde{u}_h^c\|_{L^2} - \|u_h\|_{L^2}\big| \leq \|u_h - \tilde{u}_h^c\|_{L^2} \lesssim h, \tag{4.9}$$

which implies that $\|\tilde{u}_h^c - u_h^c\|_{H^1} \lesssim h \|\tilde{u}_h^c\|_{H^1}$.

Combining (4.9), (4.8) and using the uniform boundedness of $\|G_h u_h\|_{L^2}$ one can show that

$$\|G_h u_h - \nabla u_h^c\|_{L^2} + \|u_h - u_h^c\|_{L^2} \lesssim h \tag{4.10}$$

holds for sufficiently small $h > 0$. Therefore, $\|\nabla u_h^c\|_{L^2}$ and $\|u_h^c\|_{L^2}$ are uniformly bounded. By the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, $\|u_h^c\|_{L^6}$ and $\|u_h^c\|_{L^4}$ are also uniformly bounded, which implies that

$$\begin{aligned} E_h - \mathcal{E}_h^*(u_h^c) =& \frac{1}{2}(G_h u_h - \nabla u_h^c, G_h u_h + \nabla u_h^c)_{L^2} + \frac{1}{2}(\pi_h V(u_h - u_h^c), u_h + u_h^c)_{L^2} \\ &+ \frac{\kappa}{4}(\|u_h\|_{L^4}^4 - \|u_h^c\|_{L^4}^4) \to 0 \end{aligned} \tag{4.11}$$

and

$$|\mathcal{E}_h^*(u_h^c) - \mathcal{E}(u_h^c)| = \frac{1}{2}|((\pi_h V - V)u_h^c, u_h^c)_{L^2}| \lesssim \|V - \pi_h V\|_{L^2} \to 0. \tag{4.12}$$

The inequality $E_h^* \leq \mathcal{E}_h^*(u_h^c)$, the lower bound (4.7) and (4.11) imply that

$$0 \geq E_h^* - \mathcal{E}_h^*(u_h^c) \geq E_h\big(1 - 4h^2\pi^{-2}E_h^*\big) - \mathcal{E}_h^*(u_h^c) \to 0,$$

which together with (4.6) and (4.12) gives that

$$|E - \mathcal{E}(u_h^c)| \leq |E - E_h^*| + |E_h^* - \mathcal{E}_h^*(u_h^c)| + |\mathcal{E}_h^*(u_h^c) - \mathcal{E}(u_h^c)| \to 0. \tag{4.13}$$

Assuming that $(u, u_h^c)_{L^2} \geq 0$ holds for h sufficiently small one can show that $\|u - u_h^c\|_{H^1} \to 0$ using (4.13) and similar arguments as in the proof of (Cancès *et al.*, 2010, Thm. 1). Otherwise, one can proceed with $v_h^c := -u_h^c$, which similarly yields that $\|u - v_h^c\|_{H^1} \to 0$. Since on the one hand $\|u + u_h\|_{L^2} \le \|u - v_h^c\|_{L^2} + \|u_h^c - u_h\|_{L^2} \to 0$ and on the other hand $\|u + u_h\|_{L^2}^2 = 2 + 2(u, u_h)_{L^2} \ge 2$, we get a contradiction which shows that it must hold that $(u, u_h^c)_{L^2} \ge 0$ for h sufficiently small.

The convergence of the energies, i.e., $E_h \to E$, follows immediately combining (4.11) to (4.13). To show the L^2-convergence of the gradient we use the triangle inequality to obtain that

$$\|G_h u_h - \nabla u\|_{L^2} \le \|G_h u_h - \nabla u_h^c\|_{L^2} + \|\nabla u_h^c - \nabla u\|_{L^2} \to 0.$$

Similarly, one can show that $\|u - u_h\|_{L^2} \to 0$. For the eigenvalues, we get that

$$|\lambda_h - \lambda| \le 2|E_h - E| + \frac{\kappa}{2}\big|\|u_h\|_{L^4}^4 - \|u\|_{L^4}^4\big| \to 0. \tag{4.14}$$

Algebraic manipulations and the application of Hölder's inequality for the second term on the right-hand side prove the convergence of the ground state eigenvalue approximation. This concludes the proof. ☐

The following corollary is an immediate consequence of the previous proof.

Corollary 4.4. (Uniform boundedness) It holds that $\|G_h u_h\|_{L^2}$, $\|u_h\|_{L^\infty}$, λ_h and E_h are uniformly bounded with respect to h.

For the quantification of the rates of convergence we introduce some new notation. We denote pairs of functions in $L^2(\Omega) \times H(\mathrm{div}, \Omega)$ by boldface Roman capital letters, e.g., $\mathbf{U}$, $\mathbf{V}$ and $\mathbf{W}$. The discrete analogues in $U_h \times \Sigma_h$ are denoted by $\mathbf{U}_h$, $\mathbf{V}_h$ and $\mathbf{W}_h$. Furthermore, we define the bilinear form B_u acting on the pairs $\mathbf{V} = (v, \tau)$ and $\mathbf{W} = (w, \vartheta)$ as follows:

$$B_u(\mathbf{V}, \mathbf{W}) := (\tau, \vartheta)_{L^2} + (\mathrm{div}\,\vartheta, v)_{L^2} - (\mathrm{div}\,\tau, w)_{L^2} + (Vv, w)_{L^2} + \kappa(|u|^2 v, w)_{L^2},$$

where u denotes the ground state. By rewriting (1.1) as a Poisson problem with the L^2-right-hand side $\lambda u - Vu - \kappa|u|^2 u$ and using the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$ for $d \le 3$, classical elliptic regularity theory (see, e.g., (Hackbusch, 2003, Thm. 9.1.22)) easily shows that the ground state u is H^2-regular, i.e., $u \in H^2(\Omega) \cap H_0^1(\Omega)$. The embedding $H^2(\Omega) \hookrightarrow C^0(\overline{\Omega})$ for $d \le 3$ then shows that u is essentially bounded, i.e., its L^∞-norm is finite. This in turn shows that the bilinear form B_u is well defined.

Similarly, denoting the ground state eigenvalue by λ, we define the bilinear form $J_{u,\lambda}$ by

$$J_{u,\lambda}(\mathbf{V}, \mathbf{W}) := B_u(\mathbf{V}, \mathbf{W}) - \lambda(v, w)_{L^2} + 2\kappa(|u|^2 v, w)_{L^2}.$$

We can then prove the following preliminary result.

Lemma 4.5. (Almost coercivity of $J_{u,\lambda}$) For any $\mathbf{V}_h = (v_h, G_h v_h)$ it holds that

$$\|G_h v_h\|_{L^2}^2 + \|v_h\|_{L^2}^2 \lesssim J_{u,\lambda}(\mathbf{V}_h, \mathbf{V}_h) + h^2\|\mathrm{div}\, G_h v_h\|_{L^2}^2,$$

where the hidden constant depends on the domain, the mesh regularity, the coefficients V and κ, the ground state u and the eigenvalue λ.

Proof. By Lemma A.1 there exists for any $\mathbf{V}_h = (v_h, G_h v_h)$ a pair $\mathbf{V}_h^c = (v_h^c, \nabla v_h^c)$ with $v_h^c \in H^2(\Omega) \cap H_0^1(\Omega)$ such that it holds

$$\|G_h v_h - \nabla v_h^c\|_{L^2} + \|v_h - v_h^c\|_{L^2} \lesssim h\|\operatorname{div} G_h v_h\|_{L^2}. \tag{4.15}$$

Using (Cancès *et al.*, 2010, Lem. 1), which provides a lower bound of $J_{u,\lambda}$ for conforming functions, we obtain that

$$\begin{aligned}\|G_h v_h\|_{L^2}^2 + \|v_h\|_{L^2}^2 &\lesssim \|\nabla v_h^c\|_{L^2}^2 + \|v_h^c\|_{L^2}^2 + h^2\|\operatorname{div} G_h v_h\|_{L^2}^2\\ &\lesssim J_{u,\lambda}(\mathbf{V}_h^c, \mathbf{V}_h^c) + h^2\|\operatorname{div} G_h v_h\|_{L^2}^2.\end{aligned}$$

The desired result does not include the conforming counterpart $\mathbf{V}_h^c$, but $\mathbf{V}_h$. To go back to the original function $\mathbf{V}_h$ we use (4.15), the L^∞-bound for u and Young's inequality to get that

$$\begin{aligned}&|J_{u,\lambda}(\mathbf{V}_h^c, \mathbf{V}_h^c) - J_{u,\lambda}(\mathbf{V}_h, \mathbf{V}_h)|\\ &\quad\le |(\nabla v_h^c, \nabla v_h^c - G_h v_h)_{L^2}| + |(G_h v_h, \nabla v_h^c - G_h v_h)_{L^2}|\\ &\qquad + |((V + 3\kappa u^2 - \lambda)(v_h^c - v_h), v_h^c + v_h)_{L^2}|\\ &\quad\lesssim h\|\operatorname{div} G_h v_h\|_{L^2}\big(h\|\operatorname{div} G_h v_h\|_{L^2} + \|G_h v_h\|_{L^2} + \|v_h\|_{L^2}\big)\\ &\quad\le h^2\left(1 + \frac{1}{4\epsilon}\right)\|\operatorname{div} G_h v_h\|_{L^2}^2 + \epsilon\big(\|G_h v_h\|_{L^2}^2 + \|v_h\|_{L^2}^2\big),\end{aligned}$$

which holds for all $\epsilon > 0$. Combining the previous two estimates yields

$$\begin{aligned}&\|G_h v_h\|_{L^2}^2 + \|v_h\|_{L^2}^2\\ &\quad\le C\left(J_{u,\lambda}(\mathbf{V}_h, \mathbf{V}_h) + h^2\left(1 + \frac{1}{4\epsilon}\right)\|\operatorname{div} G_h v_h\|_{L^2}^2 + \epsilon\big(\|G_h v_h\|_{L^2}^2 + \|v_h\|_{L^2}^2\big)\right)\end{aligned}$$

for some constant $C > 0$, which depends on the domain, the mesh regularity, the coefficients V and κ, the ground state u and the eigenvalue λ, but is independent of h and v_h. By choosing $\epsilon = \frac{1}{2C}$, the rightmost term can be absorbed into the left-hand side. This completes the proof. $\square$

Let $\mathbf{U} = (u, \sigma)$ and $\mathbf{U}_h = (u_h, \sigma_h)$ denote solutions of (4.1) and (4.2), respectively. Recall that we assume $(u, u_h)_{L^2} \ge 0$ so that u and u_h have compatible signs. To simplify the notation, we introduce the L^2-norm in the product space for any $\mathbf{V} = (v, \tau)$ as $\|\mathbf{V}\|^2 := \|v\|_{L^2}^2 + \|\tau\|_{L^2}^2$. Let us define the pair $\tilde{\mathbf{W}}_h = (\tilde{w}_h, \tilde{\vartheta}_h)$ as the solution to

$$(\tilde{\vartheta}_h, \tau_h)_{L^2} + (\operatorname{div} \tau_h, \tilde{w}_h)_{L^2} = 0 \qquad \text{for all } \tau_h \in \Sigma_h, \tag{4.16a}$$

$$(\operatorname{div} \tilde{\vartheta}_h, v_h)_{L^2} = (\Delta u, v_h)_{L^2} \qquad \text{for all } v_h \in U_h \tag{4.16b}$$

and set $\mathbf{W}_h = (w_h, \vartheta_h) = \tilde{\mathbf{W}}_h/\|\tilde{w}_h\|_{L^2}$. To prove an error estimate for $\|\mathbf{U} - \mathbf{U}_h\|$ we use the triangle inequality and examine the two errors $\|\mathbf{U} - \mathbf{W}_h\|$ and $\|\mathbf{U}_h - \mathbf{W}_h\|$ individually.

LEMMA 4.6. (Estimate of first term) For $h > 0$ sufficiently small it holds that

$$\|\mathbf{U} - \mathbf{W}_h\| \lesssim h,$$

where the hidden constant depends on the domain, the mesh regularity and the ground state u.

Proof. A standard *a priori* error estimate, cf. (Boffi *et al.*, 2013, Prop. 7.1.2), shows that

$$\|\tilde{\vartheta}_h - \nabla u\|_{L^2} + \|\tilde{w}_h - u\|_{L^2} \lesssim h\|u\|_{H^2}$$

since $(\tilde{w}_h, \tilde{\vartheta}_h)$ is the mixed Galerkin projection of $(u, \nabla u)$. The desired estimate then immediately follows from $\|u\|_{L^2} = 1$ and $|\|\tilde{w}_h\|_{L^2} - 1| \lesssim h$. □

The following lemma is the final step towards the desired error estimate.

LEMMA 4.7. (Estimate of second term) For $h > 0$ sufficiently small we have that

$$\|\mathbf{U}_h - \mathbf{W}_h\| \lesssim \|(u_h - u)^2\|_{L^3} + h\|u_h - u\|_{L^2} + h,$$

where the hidden constant depends on the domain, the mesh regularity, the coefficients V and κ, the ground state u and the eigenvalue λ.

Proof. We abbreviate $\mathbf{Y}_h := \mathbf{U}_h - \mathbf{W}_h$ and $y_h := u_h - w_h$. Using Lemma 4.5 we obtain that

$$\|\mathbf{U}_h - \mathbf{W}_h\|^2 \lesssim J_{u,\lambda}(\mathbf{U}_h - \mathbf{W}_h, \mathbf{U}_h - \mathbf{W}_h) + h^2\|\mathrm{div}(\sigma_h - \vartheta_h)\|_{L^2}^2 = \Xi_1 + \Xi_2 + \Xi_3,$$

where we set

$$\Xi_1 := J_{u,\lambda}(\mathbf{U}_h - \mathbf{U}, \mathbf{Y}_h), \quad \Xi_2 := J_{u,\lambda}(\mathbf{U} - \mathbf{W}_h, \mathbf{Y}_h), \quad \Xi_3 := h^2\|\mathrm{div}(\sigma_h - \vartheta_h)\|_{L^2}^2.$$

The term Ξ_1 is rewritten as follows:

$$\begin{aligned}
\Xi_1 &= B_u(\mathbf{U}_h - \mathbf{U}, \mathbf{Y}_h) - \lambda(u_h - u, y_h)_{L^2} + 2\kappa(u^2(u_h - u), y_h)_{L^2} \\
&= \lambda_h(u_h, y_h)_{L^2} - \kappa((u_h^2 - u^2)u_h, y_h)_{L^2} - \lambda(u, y_h)_{L^2} \\
&\quad - \lambda(u_h - u, y_h)_{L^2} + 2\kappa(u^2(u_h - u), y_h)_{L^2} \\
&= \frac{1}{2}(\lambda_h - \lambda)\|y_h\|_{L^2}^2 - \kappa((u_h^2 - u^2)u_h, y_h)_{L^2} + 2\kappa(u^2(u_h - u), y_h)_{L^2} \\
&= \frac{1}{2}(\lambda_h - \lambda)\|y_h\|_{L^2}^2 - \kappa((u_h - u)^2(u_h + 2u), y_h)_{L^2},
\end{aligned}$$

where we use that $(u_h, y_h)_{L^2} = (u_h, u_h - w_h)_{L^2} = \frac{1}{2}\|u_h - w_h\|_{L^2}^2$, and that (u, σ) and (u_h, σ_h) solve (4.1) and (4.2), respectively. Using that $\|u_h + 2u\|_{L^6} \lesssim \|G_h u_h\|_{L^2} + \|\nabla u\|_{L^2} \lesssim 1$ (cf. Lemma A.4) we then obtain the following estimate for Ξ_1:

$$|\Xi_1| \lesssim |\lambda_h - \lambda|\|y_h\|_{L^2}^2 + \|(u_h - u)^2\|_{L^3}\|y_h\|_{L^2}.$$

For the term Ξ_2 we get that

$$
\begin{aligned}
\Xi_2 &= B_u(\mathbf{U} - \mathbf{W}_h, \mathbf{Y}_h) - \lambda(u - w_h, y_h)_{L^2} + 2\kappa(u^2(u - w_h), y_h)_{L^2} \\
&= (\sigma - \vartheta_h, \sigma_h - \vartheta_h)_{L^2} + (\operatorname{div}(\sigma_h - \vartheta_h), u - w_h)_{L^2} - (\operatorname{div}(\sigma - \vartheta_h), y_h)_{L^2} \\
&\quad + ((V + 3\kappa u^2 - \lambda)(u - w_h), y_h)_{L^2} \\
&= (\operatorname{div}(\vartheta_h - \tilde{\vartheta}_h), y_h)_{L^2} + ((V + 3\kappa u^2 - \lambda)(u - w_h), y_h)_{L^2} \\
&= -\left(1 - \frac{1}{\|\tilde{w}_h\|_{L^2}}\right)((V + \kappa u^2 - \lambda)u, y_h)_{L^2} + ((V + 3\kappa u^2 - \lambda)(u - w_h), y_h)_{L^2},
\end{aligned}
$$

where we used that $(\operatorname{div}(\sigma - \tilde{\vartheta}_h), y_h)_{L^2} = 0$ and $\Delta u = \kappa u^3 + Vu - \lambda u$, as well as the identity $(\sigma - \vartheta_h, \sigma_h - \vartheta_h)_{L^2} + (\operatorname{div}(\sigma_h - \vartheta_h), u - w_h)_{L^2} = 0$, which is derived by integrating by parts and using (4.16a). The estimate $|\|\tilde{w}_h\|_{L^2} - 1| \lesssim h$ then allows us to bound Ξ_2 as follows:

$$
|\Xi_2| \lesssim h\|y_h\|_{L^2} + \|u - w_h\|_{L^2}\|y_h\|_{L^2}.
$$

For the term Ξ_3 we note that

$$
\operatorname{div}\sigma_h = \pi_h\big(\kappa u_h^3 + Vu_h - \lambda_h u_h\big), \qquad \operatorname{div}\vartheta_h = \pi_h\big(\kappa u^3 + Vu - \lambda u\big)/\|\tilde{w}_h\|_{L^2},
$$

where $\Delta u = \kappa u^3 + Vu - \lambda u$. This gives us

$$
\begin{aligned}
\operatorname{div}(\sigma_h - \vartheta_h) = \pi_h\bigg(&\kappa(u_h - u)(u_h^2 + u_h u + u^2) + V(u_h - u) - \lambda(u_h - u) \\
&+ (\lambda - \lambda_h)u_h + \left(1 - \frac{1}{\|\tilde{w}_h\|_{L^2}}\right)\Delta u\bigg).
\end{aligned}
$$

Using the L^2-stability of π_h the (uniform) L^∞-bounds for u and u_h (cf. Corollary 4.4), $\|u_h\|_{L^2} = 1$, and that $|\|\tilde{w}_h\|_{L^2} - 1| \lesssim h$ yields that

$$
\Xi_3 \lesssim h^2\big(\|u_h - u\|_{L^2}^2 + |\lambda - \lambda_h|^2 + h^2\big).
$$

Combining the above estimates for Ξ_1, Ξ_2 and Ξ_3, we obtain that

$$
\begin{aligned}
\|\mathbf{U}_h - \mathbf{W}_h\|^2 \lesssim{}& \big(\|(u_h - u)^2\|_{L^3} + \|u - w_h\|_{L^2} + h\big)\|y_h\|_{L^2} \\
&+ h^2\big(\|u_h - u\|_{L^2}^2 + |\lambda - \lambda_h|^2 + h^2\big),
\end{aligned}
$$

where we absorbed the term $|\lambda_h - \lambda|\|y_h\|_{L^2}^2$ into the left-hand side, which is possible for sufficiently small $h > 0$; see Theorem 4.3. Using Lemma 4.6 and the weighted Young's inequality we obtain that

$$
\|\mathbf{U}_h - \mathbf{W}_h\| \lesssim \|(u_h - u)^2\|_{L^3} + h + h\|u_h - u\|_{L^2} + h|\lambda - \lambda_h| + h^2.
$$

The assertion then follows from the uniform boundedness of λ_h (see Corollary 4.4) and from the fact that $h^2 \lesssim h$ for $h > 0$ sufficiently small. □

The following theorem gives an error estimate for the ground state, energy and eigenvalue approximations of the proposed mixed finite element discretization. It is derived by combining the two previous lemmas. For a second-order estimate for the eigenvalue approximation, which holds under additional regularity assumptions on V, we refer to Theorem 4.9.

THEOREM 4.8. (*A priori* error estimates) For sufficiently small $h > 0$ it holds that

$$\|\mathbf{U} - \mathbf{U}_h\| \lesssim h, \qquad \|\mathrm{div}(\sigma - \sigma_h)\|_{L^2} \lesssim h + \|Vu - \pi_h(Vu)\|_{L^2}. \tag{4.17}$$

The eigenvalue and energy approximations satisfy

$$|E - E_h| \lesssim h^2 + h\|V - \pi_h V\|_{L^2}, \qquad |\lambda - \lambda_h| \lesssim h. \tag{4.18}$$

If, in addition, V is $\mathcal{T}_h$-piecewise constant or H^1-regular, we have that

$$\|\mathrm{div}(\sigma - \sigma_h)\|_{L^2} \lesssim h, \qquad |E - E_h| \lesssim h^2. \tag{4.19}$$

The hidden constants in the above estimates depend on the domain, the mesh regularity, the coefficients V and κ, the ground state u and the eigenvalue λ.

Proof. By the triangle inequality and Lemma 4.6 and 4.7 we obtain that

$$\begin{aligned}\|\mathbf{U} - \mathbf{U}_h\| &\le \|\mathbf{U} - \mathbf{W}_h\| + \|\mathbf{U}_h - \mathbf{W}_h\| \\ &\lesssim \|(u_h - u)^2\|_{L^3} + h\|u_h - u\|_{L^2} + h.\end{aligned}$$

For $h > 0$ sufficiently small the term $h\|u_h - u\|_{L^2}$ is absorbed into the left-hand side, which yields that

$$\|\mathbf{U} - \mathbf{U}_h\| \lesssim \|(u_h - u)^2\|_{L^3} + h.$$

It only remains to bound the first term on the right-hand side. Elementary algebraic manipulations and the triangle inequality show that

$$\|(u_h - u)^2\|_{L^3} = \|u_h - u\|_{L^6}^2 \lesssim \|u_h - \pi_h u\|_{L^6}^2 + \|u - \pi_h u\|_{L^6}^2. \tag{4.20}$$

For the first term on the right-hand side of (4.20) we get with Lemmas A.4 and 2.1 and the triangle inequality that

$$\begin{aligned}\|u_h - \pi_h u\|_{L^6}^2 \lesssim \|G_h(u_h - \pi_h u)\|_{L^2}^2 &\le \|G_h u_h - \nabla u\|_{L^2}^2 + \|\nabla u - \Pi_h \nabla u\|_{L^2}^2 \\ &\lesssim \|\mathbf{U} - \mathbf{U}_h\|^2 + h^2,\end{aligned} \tag{4.21}$$

where we used the classical approximation property

$$\|\nabla u - \Pi_h \nabla u\|_{L^2} \lesssim h\|u\|_{H^2};$$

see, e.g., (Boffi *et al.*, 2013, Prop. 2.5.4). The second term on the right-hand side of (4.20) is bounded using Poincaré's inequality (Gilbarg & Trudinger, 2001, Eq. (7.45)) and applying the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$ for $d \leq 3$ to the gradient of u. This results in

$$\|u - \pi_h u\|_{L^6}^2 \lesssim h^2 \|\nabla u\|_{L^6}^2 \lesssim h^2 \|u\|_{H^2}^2. \tag{4.22}$$

Combining the previous estimates we obtain that

$$\|\mathbf{U} - \mathbf{U}_h\| \lesssim \|\mathbf{U} - \mathbf{U}_h\|^2 + h^2 + h.$$

By the convergence result of Theorem 4.3 the term $\|\mathbf{U} - \mathbf{U}_h\|^2$ converges to zero. Since it is a higher order term it is absorbed in the left-hand side for sufficiently small $h > 0$. Under this smallness condition it also holds that $h^2 \lesssim h$. The desired estimate for $\|\mathbf{U} - \mathbf{U}_h\|$ follows immediately.

The estimate for $|E - E_h|$ is an immediate consequence of Lemma 4.1, the argument used in (4.20) and the uniform L^∞-boundedness of u_h, cf. Corollary 4.4. For proving the eigenvalue approximation result (4.18), one may proceed similarly as in (4.14) using the convergence results for $\|\mathbf{U} - \mathbf{U}_h\|$ and $|E - E_h|$, cf. (4.17) and (4.18).

Let us next prove the estimate for $\|\operatorname{div}(\sigma - \sigma_h)\|_{L^2}$. We note that

$$\operatorname{div} \sigma_h = \pi_h\big(\kappa u_h^3 + V u_h - \lambda_h u_h\big), \qquad \operatorname{div} \sigma = \kappa u^3 + V u - \lambda u, \tag{4.23}$$

which implies that

$$\begin{aligned} \operatorname{div}(\sigma_h - \sigma) = {} & \pi_h(\kappa(u_h^3 - u^3) + V(u_h - u) - \lambda(u_h - u) - (\lambda_h - \lambda)u_h) \\ & + (\kappa(\pi_h u^3 - u^3) + \pi_h(Vu) - Vu - \lambda(\pi_h u - u)). \end{aligned}$$

The desired estimate follows immediately using (2.3), the first estimate in (4.18) and (4.17). Finally, estimate (4.19) is a direct consequence of (4.18) and (4.17). □

For H^1-regular potentials, the following theorem proves a second-order convergence result for the eigenvalue approximation.

THEOREM 4.9. (Improved error estimate) Let $V \in H^1(\Omega)$ and assume that Ω is a d-dimensional brick. Then, for sufficiently small $h > 0$ it holds that

$$\|u - u_h\|_{H^{-1}} \lesssim h^2, \qquad |\lambda - \lambda_h| \lesssim h^2, \tag{4.24}$$

where the hidden constant depends on the domain, the mesh regularity, the coefficients V and κ, the ground state u and the eigenvalue λ.

Proof. We begin with the proof of the H^{-1}-norm estimate. For mixed finite elements, such error estimates were introduced in Douglas & Roberts (1985). In the following, we use this well-known technique with the auxiliary dual problem of (Cancès *et al.*, 2010, Eq. (70)). Given a test function $w \in H_0^1(\Omega)$, it seeks $z \in H_0^1(\Omega)$ such that

$$-\Delta z + (V + 3\kappa u^2 - \lambda)z = 2\kappa(u^3, z)_{L^2} u + w - (w, u)_{L^2} u \tag{4.25}$$

holds in $H^{-1}(\Omega)$. This problem is solved by the unique solution $z \in u^\perp := \{v \in H_0^1(\Omega) : (u, v)_{L^2} = 0\} \subset H_0^1(\Omega)$ satisfying

$$(\nabla z, \nabla v)_{L^2} + ((V + 3\kappa u^2 - \lambda)z, v)_{L^2} = (w, v)_{L^2} \qquad \text{for all } v \in u^\perp.$$

The well-posedness of the latter problem is a consequence of the Lax-Milgram theorem using the coercivity of the bilinear form on the left-hand side, cf. (Cancès *et al.*, 2010, Lem. 1), and the fact that $u^\perp$ is a complete subspace of $H_0^1(\Omega)$. Assuming that $V \in H^1(\Omega)$, elliptic regularity theory implies that $z \in H^3(\Omega)$ with the estimate $\|z\|_{H^3} \lesssim \|w\|_{H^1}$. To prove the H^3-regularity, we recall the assumption that Ω is a d-dimensional brick and apply a prolongation by reflection argument, noting that the right-hand side of (4.25) satisfies zero Dirichlet boundary conditions; see (Cancès *et al.*, 2010, p. 107) for more details.

Considering the mixed form of problem (4.25), the pair (z, φ) satisfies

$$(\varphi, \tau)_{L^2} + (\operatorname{div} \tau, z)_{L^2} = 0 \qquad \text{for all } \tau \in H(\operatorname{div}, \Omega), \tag{4.26a}$$

$$(\operatorname{div} \varphi, v)_{L^2} - ((V + 3\kappa u^2 - \lambda)z, v)_{L^2} = (f, v)_{L^2} \qquad \text{for all } v \in L^2(\Omega) \tag{4.26b}$$

for the source term

$$f := -2\kappa(u^3, z)_{L^2} u - w + (w, u)_{L^2} u.$$

To derive the desired H^{-1}-norm estimate, we fix a test function $w \in H_0^1(\Omega)$ and test (4.26b) with $u_h - u \in L^2(\Omega)$ and (4.26a) with $\sigma_h - \sigma \in H(\operatorname{div}, \Omega)$ and add up the equations. After rearranging the terms, we obtain that

$$(u - u_h, w)_{L^2} = \Xi_1 + \Xi_2$$

with the expressions

$$\begin{aligned}
\Xi_1 &:= (\varphi, \sigma_h - \sigma)_{L^2} + (\operatorname{div}(\sigma_h - \sigma), z)_{L^2} + (\operatorname{div} \varphi - (V + 3\kappa u^2 - \lambda)z, u_h - u)_{L^2},\\
\Xi_2 &:= 2\kappa(u^3, z)_{L^2}(u, u_h - u)_{L^2} - (w, u)_{L^2}(u, u_h - u)_{L^2}.
\end{aligned}$$

In the following, we will add and subtract the term $\tilde{\Xi}_1$ defined by

$$\tilde{\Xi}_1 := (\varphi_h, \sigma_h - \sigma)_{L^2} + (\operatorname{div}(\sigma_h - \sigma), z_h)_{L^2} + (\operatorname{div} \varphi_h - (V + 3\kappa u^2 - \lambda)z_h, u_h - u)_{L^2}$$

with $(z_h, \varphi_h) := (\pi_h z, G_h \pi_h z)$. Let us first show that $|\tilde{\Xi}_1|$ is in fact a second-order term, i.e., $|\tilde{\Xi}_1| \lesssim h^2 \|w\|_{H^1}$. To see this, we seek a different representation of $\tilde{\Xi}_1$. Adding up (4.1a) tested with φ_h and

(4.1b) tested with z_h yields that

$$(\sigma, \varphi_h)_{L^2} + (\operatorname{div}\varphi_h, u)_{L^2} + (\operatorname{div}\sigma, z_h)_{L^2} - ((V+\kappa u^2)u, z_h)_{L^2} = -\lambda(u, z_h)_{L^2}.$$

Similarly, we get by adding up (4.2a) tested with φ_h and (4.2b) tested with z_h that

$$(\sigma_h, \varphi_h)_{L^2} + (\operatorname{div}\varphi_h, u_h)_{L^2} + (\operatorname{div}\sigma_h, z_h)_{L^2} - ((V+\kappa u_h^2)u_h, z_h)_{L^2} = -\lambda_h(u_h, z_h)_{L^2}.$$

Using these identities we can rewrite $\tilde{\Xi}_1$ as

$$\tilde{\Xi}_1 = \kappa((u_h^2 + u_h u - 2u^2)(u_h - u), z_h)_{L^2} + (\lambda - \lambda_h)(u_h, z_h)_{L^2}. \tag{4.27}$$

Since it holds that $(u_h^2 + u_h u - 2u^2)(u_h - u) = (u_h + 2u)(u_h - u)^2$, we obtain for the first term on the right-hand side of the previous equation that

$$|((u_h^2 + u_h u - 2u^2)(u_h - u), z_h)_{L^2}| \lesssim \|(u_h - u)^2\|_{L^3}\|z_h\|_{L^2} \lesssim h^2\|w\|_{H^1},$$

where we proceeded similarly as in (4.20) and used Lemma A.4. For the second term on the right-hand side of (4.27) we get with $(z, u)_{L^2} = 0$ that

$$(\lambda_h - \lambda)(u_h, z_h)_{L^2} = (\lambda_h - \lambda)(u_h - u, z_h)_{L^2} - (\lambda_h - \lambda)(u, z - z_h)_{L^2},$$

which, using (2.3), (4.18) and (4.17), yields that

$$|(\lambda_h - \lambda)(u_h, z_h)_{L^2}| \lesssim h^2\|z_h\|_{L^2} + h^2\|z\|_{H^1} \lesssim h^2\|w\|_{H^1}.$$

Let us next estimate $|\Xi_1 - \tilde{\Xi}_1|$. We use elementary algebraic manipulations to get that

$$\begin{aligned}\Xi_1 - \tilde{\Xi}_1 = {}& (\varphi - \varphi_h, \sigma_h - \sigma)_{L^2} + (\operatorname{div}(\sigma_h - \sigma), z - z_h)_{L^2} + (\operatorname{div}(\varphi - \varphi_h), u_h - u)_{L^2} \\ & - ((V + 3\kappa u^2 - \lambda)(u_h - u), z - z_h)_{L^2}.\end{aligned}$$

In the following we estimate all terms on the right-hand side separately. For the first term we get with Lemma 2.1, a classical approximation result, cf. (Boffi *et al.*, 2013, Prop. 2.5.4), and (4.17) that

$$|(\varphi - \varphi_h, \sigma_h - \sigma)_{L^2}| \le \|\varphi - \Pi_h\varphi\|_{L^2}\|\sigma - \sigma_h\|_{L^2} \lesssim h^2\|w\|_{H^1}.$$

For the second term a similar estimate can be obtained using (4.19) and (2.3).

Denoting by $I_h\colon H(\operatorname{div}, \Omega) \to \Sigma_h$ the Raviart–Thomas interpolation operator, cf. (Boffi *et al.*, 2013, Sec. 2.5.2), we obtain for the third term that

$$\begin{aligned}(\operatorname{div}(\varphi - \varphi_h), u_h - u)_{L^2} &= (\operatorname{div}(\varphi - I_h\varphi), u_h - u)_{L^2} + (\operatorname{div}(I_h\varphi - \Pi_h\varphi), u_h - u)_{L^2} \\ &= (\operatorname{div}\varphi - \pi_h \operatorname{div}\varphi, u_h - u)_{L^2} - (\varphi - I_h\varphi, \sigma - \sigma_h)_{L^2} + (\varphi - \Pi_h\varphi, \sigma - \sigma_h)_{L^2}.\end{aligned}$$

Using classical approximation results for I_h and Π_h, cf. (Boffi *et al.*, 2013, Prop. 2.5.4), and (2.3) and (4.17), we obtain the estimate

$$|(\operatorname{div}(\varphi - \varphi_h), u_h - u)_{L^2}| \lesssim h\|\mathbf{U} - \mathbf{U}_h\| \|\varphi\|_{H^2} \lesssim h^2\|w\|_{H^1}.$$

For the last term we get using (2.3) and (4.17) that

$$|((V + 3\kappa u^2 - \lambda)(u_h - u), z - z_h)_{L^2}| \lesssim h\|u - u_h\|_{L^2}\|\nabla z\|_{L^2} \lesssim h^2\|w\|_{H^1}.$$

Combining the previous estimates yields that

$$|\Xi_1 - \tilde{\Xi}_1| \lesssim h^2\|w\|_{H^1}.$$

For the term Ξ_2 we get with $(u, u_h - u)_{L^2} = -\frac{1}{2}\|u_h - u\|_{L^2}^2$ the estimate

$$|\Xi_2| \lesssim \big(\|z\|_{L^2} + \|w\|_{L^2}\big)\|u_h - u\|_{L^2}^2 \lesssim h^2\|w\|_{H^1}.$$

Using that $|(u - u_h, w)_{L^2}| \le |\tilde{\Xi}_1| + |\Xi_1 - \tilde{\Xi}_1| + |\Xi_2| \lesssim h^2\|w\|_{H^1}$ yields the desired estimate

$$\|u - u_h\|_{H^{-1}} = \sup_{w \in H_0^1(\Omega)\,:\,\|w\|_{H^1}=1} (u_h - u, w)_{L^2} \lesssim h^2.$$

Finally, to prove the second-order estimate for $|\lambda - \lambda_h|$ we introduce the notation $c := \kappa u^2 + V$ and $c_h := \kappa u_h^2 + \pi_h V$. Using the identities

$$\begin{aligned}
\|\sigma\|_{L^2}^2 &= \|\sigma - \sigma_h\|_{L^2}^2 + 2(\sigma, \sigma_h)_{L^2} - \|\sigma_h\|_{L^2}^2,\\
\|c^{1/2}u\|_{L^2}^2 &= \|c^{1/2}(u - u_h)\|_{L^2}^2 + 2(cu, u_h)_{L^2} - \|c^{1/2}u_h\|_{L^2}^2
\end{aligned}$$

and (4.1a), (4.1b), (4.2a) and (4.2b), algebraic manipulations yield that

$$\begin{aligned}
\lambda - \lambda_h &= (-\operatorname{div}\sigma + cu, u)_{L^2} - (-\operatorname{div}\sigma_h + c_h u_h, u_h)_{L^2}\\
&= \|\sigma\|_{L^2}^2 + \|c^{1/2}u\|_{L^2}^2 - \|\sigma_h\|_{L^2}^2 - \|c_h^{1/2}u_h\|_{L^2}^2\\
&= \|\sigma - \sigma_h\|_{L^2}^2 + \|c^{1/2}(u - u_h)\|_{L^2}^2\\
&\quad + 2(\sigma - \sigma_h, \sigma_h)_{L^2} + 2(cu, u_h)_{L^2} - (cu_h, u_h)_{L^2} - (c_h u_h, u_h)_{L^2}.
\end{aligned}$$

Using (4.1a), (4.2a) and (4.2b), we get that

$$\begin{aligned}
(\sigma - \sigma_h, \sigma_h)_{L^2} &= (-\operatorname{div}\sigma_h, u - u_h)_{L^2} = \lambda_h(u_h, \pi_h u - u_h)_{L^2} - (c_h u_h, \pi_h u - u_h)_{L^2}\\
&= -\frac{\lambda_h}{2}\|u - u_h\|_{L^2}^2 - (c_h u_h, u - u_h)_{L^2},
\end{aligned}$$

which yields the identity

$$\lambda - \lambda_h = \|\sigma - \sigma_h\|_{L^2}^2 + \|c^{1/2}(u - u_h)\|_{L^2}^2 - \lambda_h \|u - u_h\|_{L^2}^2 \\ + 2((c - c_h)(u - u_h), u_h)_{L^2} + ((c - c_h)u_h, u_h)_{L^2}.$$

Noting that $c - c_h = \kappa(u - u_h)(u + u_h) + V - \pi_h V$ and using (2.3) as well as the uniform L^6- and L^∞-bounds for u_h (cf. Corollary 4.4), one obtains similarly as in (4.20) that

$$|((c - c_h)(u - u_h), u_h)_{L^2}| \lesssim h^2.$$

Therefore, in order to show the second-order estimate for $|\lambda - \lambda_h|$, it only remains to consider the term

$$((c - c_h)u_h, u_h)_{L^2} = \kappa \int_\Omega (u + u_h)(u - u_h)u_h^2 \,\mathrm{d}x =: \kappa\, \Xi.$$

Regularising u_h with the averaging operator J from Lemma A.4 yields that

$$\Xi = \int_\Omega (u - u_h)(u_h - Ju_h)u_h^2 \,\mathrm{d}x + \int_\Omega (u - u_h)(Ju_h + u)(u_h^2 - (Ju_h)^2)\,\mathrm{d}x \\ + \int_\Omega (u - u_h)(Ju_h + u)(Ju_h)^2 \,\mathrm{d}x.$$

Noting that the gradient of $(Ju_h + u)(Ju_h)^2$ can be computed as

$$\nabla((Ju_h + u)(Ju_h)^2) = (3Ju_h^2 + 2uJu_h)\nabla Ju_h + (Ju_h)^2 \nabla u,$$

we obtain with Lemma A.3 and the uniform L^∞-bound of u_h that

$$\|(Ju_h + u)(Ju_h)^2\|_{H^1} \lesssim 1.$$

With this, using the uniform L^∞-bound of u_h and Ju_h, as well as the approximation error estimate $\|u_h - Ju_h\|_{L^2}$ and $\|u - u_h\|_{L^2}$, and the first estimate in (4.24), we obtain that

$$|\Xi| \lesssim h\|u - u_h\|_{L^2} + \|u - u_h\|_{H^{-1}} \lesssim h^2.$$

Combining the above estimates, the desired second-order approximation for $|\lambda - \lambda_h|$ immediately follows. □

5. Numerical experiments

Having laid the groundwork with our theoretical framework and error analysis for the mixed finite element discretization of the Gross–Pitaevskii eigenvalue problem, we now shift our focus to numerical experiments. These experiments are essential both to validate our theoretical insights and to demonstrate the practicality of our approach. For the implementation we have chosen solvers tailored to the finite-dimensional nonlinear eigenvector problem (2.2), with the goal of aligning our numerical methods with the theoretical principles previously discussed.

In the realm of suitable methods, the discrete normalised gradient flow method referenced in Bao & Du (2004) is a notable choice. This method is part of a diverse array of gradient flow approaches, each varying in their choice of metric, as indicated in Raza *et al.* (2009); Danaila & Kazemi (2010); Kazemi & Eckart (2010). An interesting advancement in this field is the introduction of an energy-adaptive metric, detailed in Henning & Peterseim (2020), which has been further analysed for quantitative errors in subsequent studies Zhang (2022); Altmann *et al.* (2022b); Chen *et al.* (2024b). Relatedly, Riemannian optimization techniques, including Riemannian conjugate gradient Antoine *et al.* (2017); Danaila & Protas (2017) and Riemannian Newton methods Altmann *et al.* (2023), offer additional avenues for exploration. Other methods that focus on the formulation of the eigenvalue problem, such as the self-consistent field (SCF) iteration Cancès (2000); Dion & Cancès (2007) and Newton's method Jarlebring & Upadhyaya (2022), also contribute valuable perspectives. It is interesting to note that assumptions about the symmetry of the condensate can lead to a reduction in the dimension of the problem, as explored in Bao & Tang (2003). Furthermore, the complexity of solving the nonlinear constraint minimization problem can be reduced by using problem-adapted basis functions with high approximation quality Henning *et al.* (2014); Henning & Persson (2023); Peterseim *et al.* (2024), using techniques from (Super-) Localized Orthogonal Decomposition Målqvist & Peterseim (2014); Hauck & Peterseim (2023).

In this paper we use the J-method of Jarlebring *et al.* (2014); Altmann *et al.* (2021) to solve the nonlinear discrete problem because, through the choice of shift, it nicely blends between the reliable linear convergence of gradient-descent type schemes and the local quadratic convergence of Newton-type methods. To apply the J-method in the mixed setting we eliminate the dual variable in (4.2). This results in a system matrix of the form $(M(u)+CB^{-1}C^T)$, where B is the Raviart–Thomas mass matrix, C is the Raviart–Thomas divergence matrix and $M(u)$ is a diagonal matrix containing the nonlinearity and the potential. To avoid the costly computation of the Schur complement when solving with the system matrix we use the Woodbury matrix identity. This gives

$$(M(u)+CB^{-1}C^T)^{-1} = M(u)^{-1} - M(u)^{-1}C(B+C^TM(u)^{-1}C)^{-1}C^TM(u)^{-1},$$

where the latter matrix is much easier to compute since $M(u)$ is diagonal. Note that since $M(u)$ is diagonal $C^TM(u)^{-1}C$ is in fact a sparse matrix. For the damping, shifting, tolerances, etc., we use a similar parameter setting as in (Altmann *et al.*, 2021, Sec. 6). In particular, we use a damping strategy with an energy-diminishing step-size control when the L^2-norm of the residuals is larger than 10^{-2}. For smaller residuals damping is disabled and shifting is enabled. At this point, the method takes about three to four iterations to converge to machine accuracy. For implementation details see the code provided at https://github.com/moimmahauck/GPE_RT0.

This section consists of two parts. First, we numerically investigate the optimal order convergence of the proposed mixed finite element discretization of the Gross–Pitaevskii problem (see Theorem 4.8 and 4.9). Second, we numerically validate the lower bounds of the ground state energy (see Theorem 3.1).

5.1 *Validation of optimal convergence rates*

To verify the optimal order convergence we consider the domain $\Omega = (-L,L)^2$ with $L = 8$ and the harmonic potential $V(x) = \frac{1}{2}|x|^2$. For this setting the ground state is point symmetric with respect to the

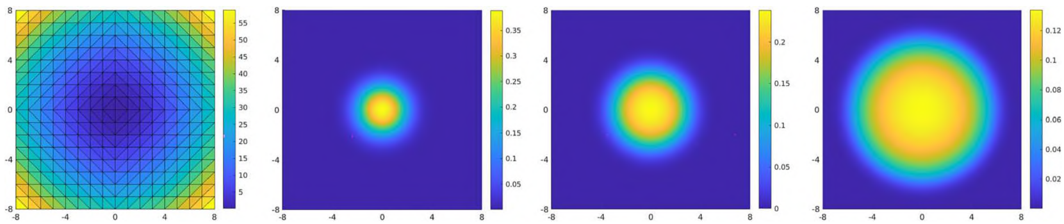

FIG. 1. Projection of the potential onto the space of piecewise constants (left) and ground states for the harmonic potential for the parameters $\kappa = 10, 100, 1000$ (second to last plot).

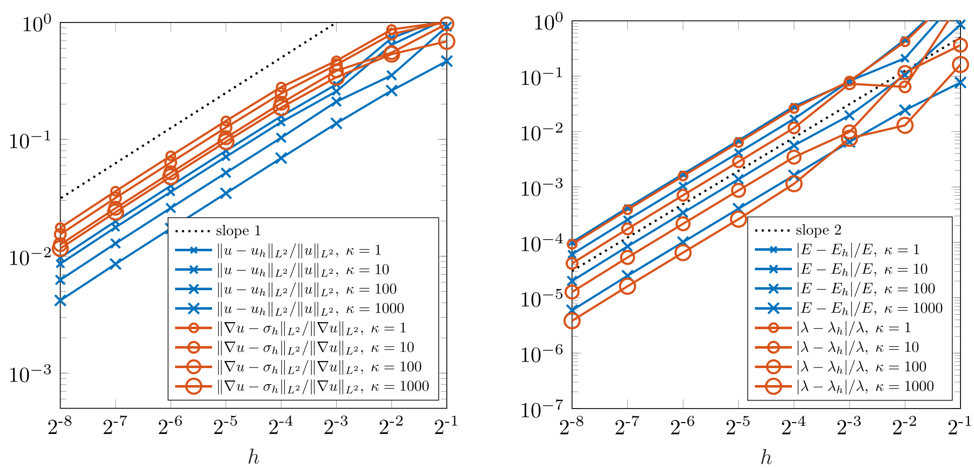

FIG. 2. Error plots of the primal and dual variables (left) and of the energy and eigenvalue (right). The expected orders of convergence are indicated by black dotted lines.

origin and decays exponentially. The decay depends on the parameter κ: the larger κ, the more repulsive the particle interaction and the more spread out the mass; see Fig. 1 (last three plots).

For the discretization, we consider a hierarchy of meshes constructed by uniform red refinement of an initial mesh. The initial mesh is constructed from a Friedrichs–Keller triangulation consisting of eight elements by rotating the triangles in the lower right and upper left squares so that the mesh is point symmetric with respect to the origin. For each mesh in the hierarchy we compute a ground state approximation, where we project the potential onto the space of piecewise constants with respect to the considered mesh; see Fig. 1 (left) for one projected potential.

Figure 2 then shows the errors of the mixed finite element discretization for several values of κ. Note that since no analytical solution is available, the errors are computed with respect to a reference solution. This reference solution is computed on a mesh obtained by twice uniform red refinement of the finest mesh in the hierarchy. One observes first-order convergence for the primal and dual variables and second-order convergence for the energies and eigenvalues. Recalling that $V \in H^1(\Omega)$, this is consistent with the predictions in Theorem 4.8 and 4.9. We observe only a weak dependence of the errors on the parameter κ. More precisely, the errors are slightly smaller for larger κ.

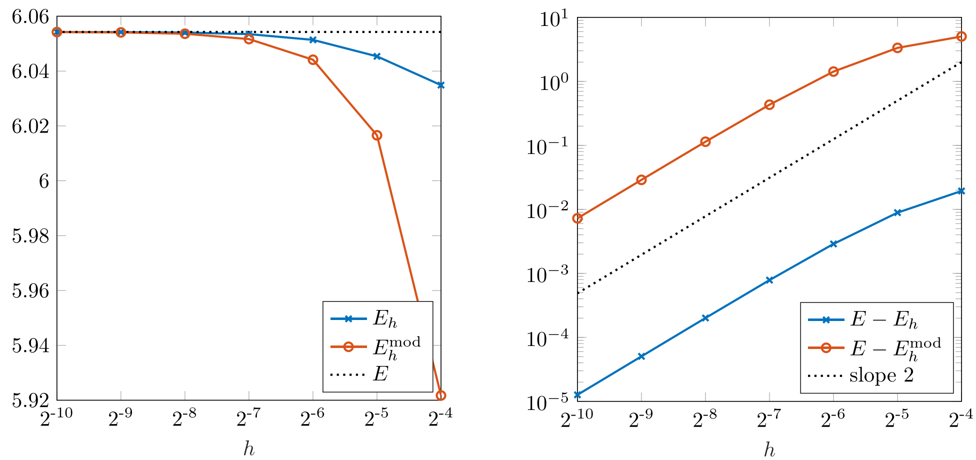

FIG. 3. Ground state energy approximations for the harmonic potential (left) and the difference between the reference energy and the energy approximations in a double-logarithmic plot (right). The blue and red curves correspond to the discrete energy and the modified discrete energy, respectively.

5.2 *Validation of lower energy bounds*

Next, we numerically verify the lower ground state energy bound given in Theorem 3.1. We consider several different settings, namely a harmonic potential, a disorder potential and a constant potential. Recall the modified discrete energy E_h^{mod} was defined as the left-hand side of (3.1). To satisfy the assumption of Theorem 3.1 that the potential is piecewise constant, we construct the potentials by prolongation of a piecewise constant potential on a coarse mesh. Reference values for the energies are computed using a $\mathcal{Q}^2$-finite element implementation together with the energy-adaptive Riemannian gradient descent method from Henning & Peterseim (2020). Note that, in order to use the same potentials for both methods we choose the potential to be piecewise constant on a Cartesian mesh. For all our numerical experiments such a Cartesian mesh is constructed by joining opposing pairs of triangles of the coarse triangulation.

5.2.1 *Harmonic potential with strong interaction.* First let us consider the harmonic potential $V(x) = \frac{1}{2}|x|^2$ and the large parameter $\kappa = 1000$. The coarse mesh used for this numerical example is shown in the background of Figure 1 (left).

In Fig. 3 (left) one observes that the discrete energy E_h and the modified discrete energy E_h^{mod} strictly increase as h is decreased, i.e., they approach the ground state energy from below. The observation was predicted for the modified discrete energy by Theorem 3.1. Figure 3 (right) shows the second order convergence of E_h and E_h^{mod} towards the reference energy and therefore also the asymptotical exactness of the lower bound. Note that, in general, the discrete energy alone is not a lower bound for the ground state energy, as the numerical example below for the constant potential shows.

5.2.2 *Disorder potential and exponential localization.* Second, we consider a disorder potential constructed using the Friedrichs–Keller triangulation shown in Fig. 4 (left). More precisely, we first join any pair of opposing triangles into squares of side length $\epsilon = 2^{-6}$. On all these squares, the coefficients is chosen to be constant, with values obtained as realizations of independent coin-flip random variables

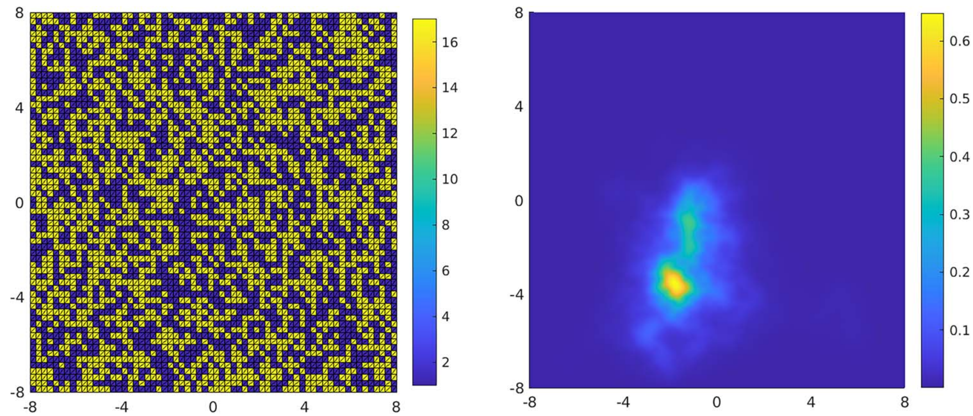

FIG. 4. Disorder potential with coarse mesh used to construct the hierarchy of meshes in the background (left). Approximation of the highly localised ground state (right).

taking the values 1 and $1 + (2\epsilon L)^{-2}$. The parameter κ is chosen to be one. For such coefficients there occurs an effect called Anderson localization (see, e.g., Altmann *et al.* (2018, 2020, 2022a) for numerical and theoretical studies). The exponential localization of the ground state can be seen in Fig. 4 (right). We emphasise that this example is numerically quite challenging, as can be seen from the comparatively large number of J-method iterations required.

For the discretization we use a hierarchy of meshes constructed by uniform refinement of the Friedrichs–Keller triangulation considered above. On each mesh of the hierarchy, the potential is obtained by prolongation.

In Fig. 5 (left) it can be observed that, also for the disorder potential, E_h and E_h^{mod} approach the ground state energy from below as the mesh size is decreased. Figure 5 (right) again demonstrates the second-order convergence of E_h and E_h^{mod} towards the reference energy.

5.2.3 *Constant potential and necessity of modification.* Third, we consider a constant potential, i.e., $V \equiv 1$. Although this choice may be unphysical, it is an example showing that the modification of the discrete energies is indeed necessary to obtain lower bounds. The parameter κ is chosen to be one. For the discretization we consider a hierarchy of meshes constructed by uniform refinement of the coarsest possible Friedrichs–Keller triangulation consisting of two elements.

In Fig. 6 (left) one observes that the discrete energies E_h approach the ground state energy from above (and not from below) as the mesh size is decreased. Nevertheless, as predicted by Theorem 3.1, the modified discrete energy E_h^{mod} is a lower bound. Figure 6 (right) shows the second-order convergence for E_h^{mod}, while $E - E_h$ is negative in this example and therefore not shown in the double-logarithmic plot. We emphasise that there are a number of numerical examples that demonstrate the need to consider a modified discrete energy. Typical features of such examples are coarse and possibly jumping coefficients and meshes with local grading; see also Gallistl (2023) for more examples in the linear setting.

6. Conclusion

In conclusion this paper has effectively demonstrated the application of a mixed finite element discretization to the Gross–Pitaevskii eigenvalue problem, with an emphasis on the computation of a lower energy

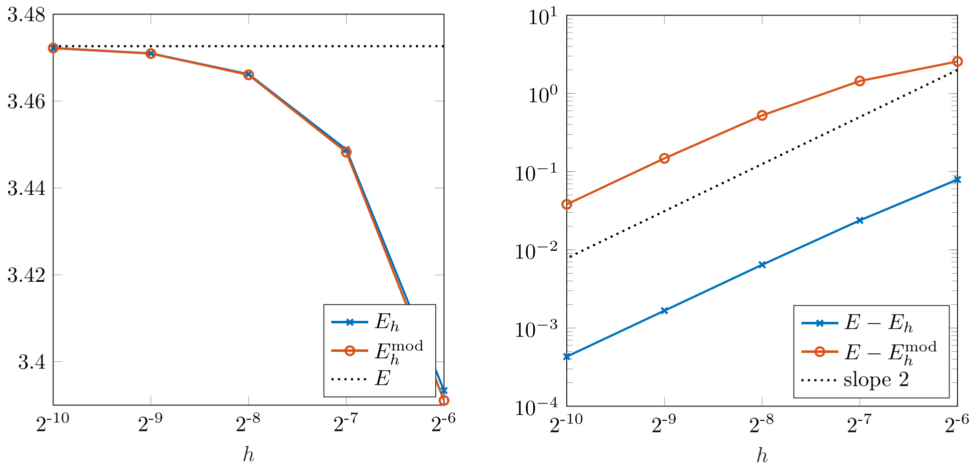

FIG. 5. Ground state energy approximations for the disorder potential (left) and the difference between the reference energy and the energy approximations in a double-logarithmic plot (right). The blue and red curves correspond to the discrete energy and the modified discrete energy, respectively.

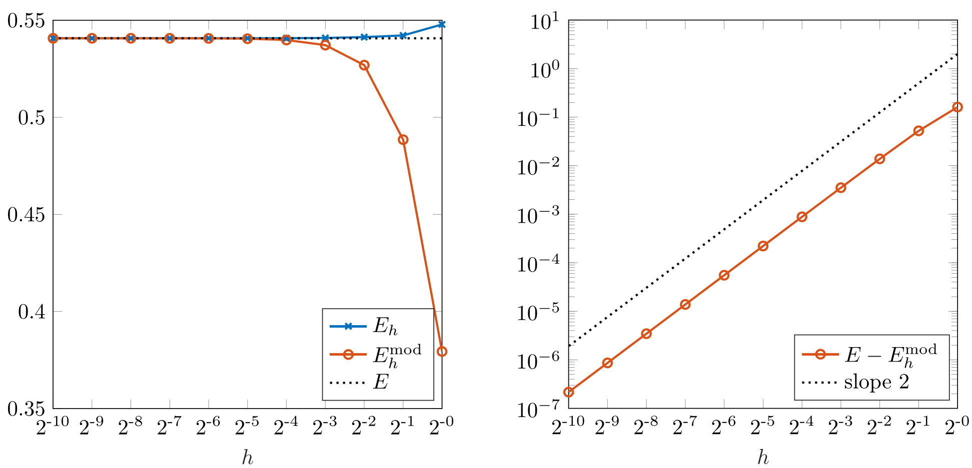

FIG. 6. Ground state energy approximations for a constant potential (left) and the difference between the reference energy and the energy approximations in a double-logarithmic plot (right). The blue and red curves correspond to the discrete energy and the modified discrete energy, respectively.

bound. Our numerical experiments have, not only validated the theoretical framework, but also confirmed the practicality of obtaining a computable lower bound on the ground state energy. This result provides a new aspect to the understanding and reliable numerical simulation of Bose–Einstein condensates.

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Appendix

A. Collection of frequently used bounds

The following lemma provides, for any discrete function, a conforming lifting with a corresponding approximation estimate.

LEMMA A.1. (Conforming lifting) For any $v_h \in U_h$ there exists $v_h^c \in H^2(\Omega) \cap H_0^1(\Omega)$ such that it holds

$$\|G_h v_h - \nabla v_h^c\|_{L^2} + \|v_h - v_h^c\|_{L^2} \lesssim h\|\operatorname{div} G_h v_h\|_{L^2}.$$

Proof. We denote by $v_h^c \in H_0^1(\Omega)$ the solution to Poisson's equation $-\Delta v_h^c = -\operatorname{div} G_h v_h$ in Ω subject to homogeneous Dirichlet boundary conditions. We emphasise that $v_h^c \in H^2(\Omega) \cap H_0^1(\Omega)$ with $\|v_h^c\|_{H^2} \lesssim \|\operatorname{div} G_h v_h\|_{L^2}$, which follows from classical elliptic regularity theory on convex domains, see, e.g., (Hackbusch, 2003, Thm. 9.1.22). The pair $(v_h, G_h v_h) \in U_h \times \Sigma_h$ is the Galerkin approximation of the mixed system and therefore satisfies the standard *a priori* error estimate

$$\|G_h v_h - \nabla v_h^c\|_{L^2} + \|v_h - v_h^c\|_{L^2} \lesssim h\|v_h^c\|_{H^2},$$

cf. (Boffi *et al.*, 2013, Prop. 7.1.2). The assertion follows immediately. □

LEMMA A.2. (L^∞-bound) Any $v_h \in U_h$ satisfies that

$$\|v_h\|_{L^\infty} \lesssim \|\operatorname{div} G_h v_h\|_{L^2}.$$

Proof. We denote by v_h^c the conforming lifting and compute

$$\|v_h\|_{L^\infty} \lesssim \|v_h - \pi_h v_h^c\|_{L^\infty} + \|\pi_h v_h^c\|_{L^\infty}.$$

The first term on the right-hand side can be controlled by an inverse estimate and the well-known superconvergence result from Douglas & Roberts (1985); Brandts (1994). One obtains that

$$\|v_h - \pi_h v_h^c\|_{L^\infty} \lesssim h^{-d/2}\|v_h - \pi_h v_h^c\|_{L^2} \lesssim h^{2-d/2}\|\operatorname{div} G_h v_h\|_{L^2}.$$

The remaining term is bounded by the H^2-norm of v_h^c, which again is controlled by $\|\operatorname{div} G_h v_h\|_{L^2}$ thanks to elliptic regularity and the Sobolev embedding. □

Given $v_h \in U_h$, we define a piecewise affine function $Jv_h \in H_0^1(\Omega)$ by assigning to each vertex z of the triangulation the arithmetic mean of the values that v_h attains at z when restricted to any elements containing z; if z is a boundary vertex, the value of Jv_h is set to zero to conform to the homogeneous boundary condition. Such averaging operators are well studied (see, e.g., Brenner & Scott (2008)) and were used in the context of mixed finite elements, e.g., in Huang & Xu (2012).

LEMMA A.3. (Averaging operator) Any $v_h \in U_h$ satisfies that

$$\|Jv_h\|_{L^\infty} \lesssim \|v_h\|_{L^\infty}$$

and

$$\|h^{-1}(v_h - Jv_h)\|_{L^2} + \|\nabla Jv_h\|_{L^2} \lesssim \|G_h v_h\|_{L^2}.$$

Proof. The first bound follows directly from the construction of the function Jv_h. Following standard arguments, cf. (Brenner & Scott, 2008, Lemma 10.6.6), we further obtain that

$$\|h^{-1}(v_h - Jv_h)\|_{L^2} + \|\nabla Jv_h\|_{L^2} \lesssim \sqrt{\sum_F h_F^{-1} \|[v_h]_F\|^2_{L^2(F)}},$$

where the sum runs over all faces F and the bracket indicates the inter-element jump across F, which is defined as the usual trace if F is a boundary face. It was shown in Lovadina & Stenberg (2006); Gao & Qiu (2018) that this term is bounded by $\|G_h v_h\|_{L^2}$. □

LEMMA A.4. (Discrete embedding) Any $v_h \in U_h$ satisfies $\|v_h\|_{L^6} \lesssim \|G_h v_h\|_{L^2}$.

Proof. Let $Jv_h \in H^1_0(\Omega)$ denote the regularization by averaging from above. From the triangle inequality, a classical comparison result between L^p-norms and the Sobolev embedding, we deduce that

$$\|v_h\|_{L^6} \lesssim \|h^{-d/3}(v_h - Jv_h)\|_{L^2} + \|\nabla Jv_h\|_{L^2}.$$

By Lemma A.3 this is controlled by $\|G_h v_h\|_{L^2}$. □

As a consequence we note the following bound

$$\|u_h\|_{L^6} + \|u_h^c\|_{L^6} \lesssim \|G_h u_h\|_{L^2} + h\|\mathrm{div}\, G_h u_h\|. \tag{A.1}$$

Proof. The bound for the first term on the left-hand side is shown in Lemma A.4. Thanks to the Sobolev embedding, we have for the second term on the left-hand side that $\|u_h^c\|_{L^6} \lesssim \|\nabla u_h^c\|_{L^2}$. With the triangle inequality and Lemma A.1 we thus obtain that

$$\|u_h^c\|_{L^6} \lesssim \|G_h u_h\|_{L^2} + h\|\mathrm{div}\, G_h u_h\|.$$

□