BIT Numerical Mathematics
https://doi.org/10.1007/s10543-020-00830-3

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A multigrid method for the ground state solution of Bose–Einstein condensates based on Newton iteration

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Received: 10 July 2020 / Accepted: 22 September 2020

Abstract
In this paper, a new kind of multigrid method is proposed for the ground state solution of Bose–Einstein condensates based on Newton iteration scheme. Instead of treating eigenvalue λ and eigenvector u separately, we regard the eigenpair (λ, u) as one element in the composite space $\mathbb{R} \times H_0^1(\Omega)$ and then Newton iteration step is adopted for the nonlinear problem. Thus in this multigrid scheme, the main computation is to solve a linear discrete boundary value problem in every refined space, which can improve the overall efficiency for the simulation of Bose–Einstein condensations.

Keywords BEC · GPE · Nonlinear eigenvalue problem · Multigrid method · Finite element method

Mathematics Subject Classification 65N30 · 65N25 · 65L15 · 65B99

1 Introduction

A Bose–Einstein condensate (BEC) is a state of a dilute gas of bosons cooled to temperature very close to absolute zero [4,21]. Under such condition, a large fraction of bosons will occupy the lowest quantum state, at which point, macroscopic quantum becomes apparent [20]. BEC was first proposed by A. Einstein who generalized a work of S. N. Bose on the quantum statistics for photons [10] to a gas of non-interacting bosons [22,23]. Then Gross-Pitaevskii (GP) theory was developed by Gross [24] and

Communicated by Marko Huhtanen.

This work was supported in part by the National Key Research and Development Program of China (2019YFA0709601), National Natural Science Foundations of China (NSFC 11771434, 11801021, 91730302, 91630201), the National Center for Mathematics and Interdisciplinary Science, CAS.

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Published online: 19 January 2021

Pitaevskii [27] independently in 1960s to describe the dynamics of a BEC [28]. Since the first experimental observation of BEC in 1995, much attention has been paid to the Gross-Pitaevskii equation (GPE) [17,26].

It is known that the wave function ψ of a sufficiently dilute condensate, in the presence of an external potential $\widetilde{W}$, satisfies the following GPE

$$\left(-\frac{\hbar^2}{2m}\Delta + \widetilde{W} + \frac{4\pi\hbar^2 aN}{m}|\psi|^2\right)\psi = \mu\psi, \tag{1}$$

where μ is the chemical potential and N is the number of atoms in the condensate. $4\pi\hbar^2 a/m$ represents the effective two-body interaction, where $\hbar$ is the Plank constant, a is the scattering length (positive for repulsive interaction and negative for attractive interaction) and m is the particle mass. In this paper, we assume the external potential $\widetilde{W}(x)$ is measurable, locally bounded and tends to infinity as $|x| \to \infty$ in the sense that

$$\inf_{|x|\geq r} \widetilde{W}(x) \to \infty \quad \text{as} \quad r \to \infty.$$

Then the wave function ψ must vanish exponentially fast as $|x| \to \infty$. Furthermore, (1) can be written as

$$\left(-\Delta + \frac{2m}{\hbar^2}\widetilde{W} + 8\pi aN|\psi|^2\right)\psi = \frac{2m\mu}{\hbar^2}\psi. \tag{2}$$

Hence in this paper, we are concerned with the smallest eigenpair for the following non-dimensionalized GPE problem:

$$\begin{cases} -\Delta u + Wu + \zeta|u|^2 u = \lambda u, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, \\ \int_\Omega |u|^2 d\Omega = 1, \end{cases} \tag{3}$$

where $\Omega \subset \mathbb{R}^d\,(d = 1, 2, 3)$ denotes the computing domain which has the cone property [1], ζ is some positive constant and $W(x) = \gamma_1 x_1^2 + \cdots + \gamma_d x_d^2 \geq 0$ with $\gamma_1, \ldots, \gamma_d > 0$ [13,32].

In the past decades, there have existed many papers discussing the numerical methods for the time-dependent GPEs and time-independent GPEs. Please refer to [2–5,11–13,15,16] and papers cited therein. Especially, in [18,32], the convergence and the priori error estimates of the finite element method for GPEs have been proved, which will be used later in this paper.

Solving such kind of nonlinear eigenvalue problem is an important but difficult problem in science and engineering computation. As is known to us all that the multigrid method provides an optimal complexity algorithm to solve discrete boundary value problems [8,14,25,29–31]. The aim of this paper is to propose a multigrid scheme for GPEs based on Newton iteration method. More precisely, GPE is regarded as a nonlinear problem in the composite space $\mathbb{R} \times H_0^1(\Omega)$ and then Newton iteration is

adopted to derive a linearized boundary value problem. Thus, we just need to solve a linear problem with finite element method in every refined space. With this multigrid scheme, solving GPE problem will not be more difficult than solving the corresponding boundary value problem. Besides, the convergence rate and computational work of this method are also analyzed in this paper.

An outline of the paper goes as follows. In Sect. 2, we introduce the finite element method and corresponding error estimates for the ground state solution of BEC, i.e. non-dimensionalized GPE. A Newton iteration method for GPE is presented in Sect. 3. In Sect. 4, we propose a type of multigrid algorithm for GPE based on Newton iteration method. Section 5 is devoted to estimating the computational work of the multigrid method designed in Sect. 4. Two numerical examples are presented in Sect. 6 to validate the theoretical analysis. Finally, some concluding remarks are given in the last section.

2 Finite element method for Gross-Pitaevskii equation

This section is devoted to introducing some notation and the finite element method for GPE problem. The letter C (with or without subscripts) denotes a generic positive constant which may be different at its different occurrences. For convenience, the symbols $\lesssim$, $\gtrsim$ and $\approx$ will be used in this paper to denote $x_1 \leq C_1 y_1$, $x_2 \geq c_2 y_2$ and $c_3 x_3 \leq y_3 \leq C_3 x_3$ for some constants C_1, c_2, c_3, C_3 that are independent of mesh sizes (see, e.g., [30]). We shall use the standard notation for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms $\|\cdot\|_{s,p,\Omega}$ and seminorms $|\cdot|_{s,p,\Omega}$ (see, e.g., [1]). For $p = 2$, we denote $H^s(\Omega) = W^{s,2}(\Omega)$, $H_0^1(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\}$, where $v|_{\partial\Omega} = 0$ is in the sense of trace and $\|\cdot\|_{s,\Omega} = \|\cdot\|_{s,2,\Omega}$. In this paper, we use $\|\cdot\|_s$ to denote $\|\cdot\|_{s,\Omega}$ for simplicity.

For the aim of finite element discretization, the corresponding weak form for (3) can be described as follows: Find $(\lambda, u) \in \mathbb{R} \times V$ such that $b(u, u) = 1$ and

$$a(u, v) = \lambda b(u, v), \quad \forall v \in V, \tag{4}$$

where $V = H_0^1(\Omega)$ and

$$a(u, v) = \int_\Omega \big(\nabla u \cdot \nabla v + W u v + \zeta |u|^2 u v\big) d\Omega, \quad b(u, v) = \int_\Omega u v d\Omega.$$

We also introduce the linearized form $a'(u; v, w)$ by

$$a'(u; v, w) = \int_\Omega \big(\nabla v \cdot \nabla w + W v w + 3\zeta |u|^2 v w\big) d\Omega, \quad \forall v, w \in V. \tag{5}$$

Here and hereafter in this paper, we only consider the smallest eigenvalue and the corresponding eigenfunction of the problem (4). For GPE problem, we can find the following estimates from [18].

Lemma 1 *There exist positive constants M, C_L and C_U such that for all $v \in H_0^1(\Omega)$,*

$$0 \le (\nabla v, \nabla v) + (Wv + \zeta |u|^2 v, v) - \lambda(v, v) \le M \|v\|_1^2 \tag{6}$$

and

$$C_L \|v\|_1^2 \le a'(u; v, v) - \lambda(v, v) \le C_U \|v\|_1^2. \tag{7}$$

Now, let us define the finite element method [9,19] for the problem (4). First we generate a shape-regular decomposition of the computing domain $\Omega \subset \mathbb{R}^d$ and the diameter of a cell $K \in \mathcal{T}_h$ is denoted by h_K. The mesh diameter h describes the maximum diameter of all cells $K \in \mathcal{T}_h$. Based on the mesh $\mathcal{T}_h$, we construct the linear finite element space denoted by $V_h \subset V$. We assume that $V_h \subset V$ satisfies the following assumption:

$$\lim_{h \to 0} \inf_{v \in V_h} \|w - v\|_1 = 0, \quad \forall w \in V. \tag{8}$$

The standard finite element method for (4) is to solve the following eigenvalue problem: Find $(\lambda_h, u_h) \in \mathbb{R} \times V_h$ such that $b(u_h, u_h) = 1$ and

$$a(u_h, v_h) = \lambda_h b(u_h, v_h), \quad \forall v_h \in V_h. \tag{9}$$

Then we define

$$\delta_h(u) := \inf_{v_h \in V_h} \|u - v_h\|_1. \tag{10}$$

The error estimates of the finite element method for (4) are presented in the following lemma which can be found in [18,32].

Lemma 2 ([18, Theorem 1]) *There exists $h_0 > 0$, such that for all $0 < h < h_0$, the smallest eigenpair approximation (λ_h, u_h) of (9) has the following error estimates*

$$\|u - u_h\|_1 \lesssim \delta_h(u), \tag{11}$$

$$\|u - u_h\|_0 \lesssim \eta_a(V_h) \|u - u_h\|_1 \lesssim \eta_a(V_h) \delta_h(u), \tag{12}$$

$$|\lambda - \lambda_h| \lesssim \|u - u_h\|_1^2 + \|u - u_h\|_0 \lesssim \eta_a(V_h) \delta_h(u), \tag{13}$$

where $\eta_a(V_h)$ is defined as follows

$$\eta_a(V_h) = \|u - u_h\|_1 + \sup_{f \in L^2(\Omega), \|f\|_0 = 1} \inf_{v_h \in V_h} \|Tf - v_h\|_1 \tag{14}$$

with the operator T being defined as follows: Find $Tf \in u^\perp$ such that

$$a'(u; Tf, v) - (\lambda(Tf), v) = (f, v), \quad \forall v \in u^\perp,$$

and $u^\perp = \left\{ v \in V : \int_\Omega uv d\Omega = 0 \right\}$.

3 Newton iteration method for Gross-Pitaevskii equation

In this section, Newton iteration method is introduced to solve the GPE problem in a composite space defined as follows:

Denote the space $\mathbb{R} \times H_0^1(\Omega)$ by X and $\mathbb{R} \times H^{-1}(\Omega)$ by X^* with the norm

$$\|(\gamma, w)\|_X = |\gamma| + \|w\|_1 \quad \text{and} \quad \|(\gamma, w)\|_0 = |\gamma| + \|w\|_0, \quad \forall (\gamma, w) \in X.$$

Similarly, the corresponding finite element space $\mathbb{R} \times V_h$ is denoted by X_h.

For any (γ, w), $(\mu, v) \in X$, we define a nonlinear operator $\mathcal{G} : X \to X^*$ as follows

$$\begin{aligned} \langle \mathcal{G}(\gamma, w), (\mu, v) \rangle = & (\nabla w, \nabla v) + (Ww + \zeta |w|^2 w - \gamma w, v) \\ & + \frac{1}{2}\mu\big(1 - \int_\Omega w^2 d\Omega\big). \end{aligned} \tag{15}$$

Since we request $\|u\|_0^2 = 1$, (4) can be rewritten as: Find $(\lambda, u) \in X$ such that

$$\langle \mathcal{G}(\lambda, u), (\mu, v) \rangle = 0, \quad \forall (\mu, v) \in X. \tag{16}$$

Then, the discrete form (9) can be rewritten as: Find $(\lambda_h, u_h) \in X_h$ such that

$$\langle \mathcal{G}(\lambda_h, u_h), (\mu_h, v_h) \rangle = 0, \quad \forall (\mu_h, v_h) \in X_h. \tag{17}$$

The Fréchet derivation of $\mathcal{G}$ at (λ, u), $\mathcal{G}'(\lambda, u) : X \to X^*$, is a bounded linear operator given by

$$\begin{aligned} \langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, v) \rangle &= (\nabla w, \nabla v) + ((W + 3\zeta u^2 - \lambda)w, v) \\ &\quad - \gamma(u, v) - \mu(u, w) \\ &= a'(u; w, v) - \lambda(w, v) - \gamma(u, v) - \mu(u, w) \\ &= \widehat{a}(\lambda, u; w, v) + \widehat{b}(u; v, \gamma) + \widehat{b}(u; w, \mu), \end{aligned} \tag{18}$$

where

$$\widehat{a}(\lambda, u; w, v) = a'(u; w, v) - \lambda(w, v), \quad \widehat{b}(u; v, \mu) = -\mu(u, v).$$

Assume we have an initial eigenpair approximation (λ', u') on the finite element space X_h, Newton iteration method for GPE is defined as follows to get a better eigenpair approximation $(\lambda'', u'') \in X_h$:

$$\langle \mathcal{G}'(\lambda', u')(\lambda'' - \lambda', u'' - u'), (\mu, v) \rangle = -\langle \mathcal{G}(\lambda', u'), (\mu, v) \rangle, \quad \forall (\mu, v) \in X_h. \tag{19}$$

From (15) and (18), (19) can be rewritten as the following mixed boundary value problem: Find $(\lambda^{''}, u^{''}) \in X_h$ such that

$$\begin{cases} \widehat{a}(\lambda^{'}, u^{'}; u^{''}, v) + \widehat{b}(u^{'}; v, \lambda^{''}) = (2\zeta(u^{'})^3 - \lambda^{'}u^{'}, v), & \forall v \in V_h, \\ \widehat{b}(u^{'}; u^{''}, \mu) = -\mu/2 - \mu(u^{'}, u^{'})/2, & \forall \mu \in \mathbb{R}. \end{cases} \tag{20}$$

The isomorphism property of $\mathcal{G}'$ is analyzed in the following theorem which also guarantees the well-posedness of the above mixed problem.

Theorem 1 *If the mesh size h is sufficiently small, then for the linearized operator $\mathcal{G}'$ presented in (18), we have*

$$\sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, v)\rangle}{\|(\mu, v)\|_X} \gtrsim \|(\gamma, w)\|_X, \quad \forall (\gamma, w) \in X, \tag{21}$$

and

$$\sup_{(\mu,v)\in X_h} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, v)\rangle}{\|(\mu, v)\|_X} \gtrsim \|(\gamma, w)\|_X, \quad \forall (\gamma, w) \in X_h. \tag{22}$$

For any $(\widehat{\lambda}, \widehat{u}) \in X$ such that $\|(\widehat{\lambda} - \lambda, \widehat{u} - u)\|_X$ is small enough, there holds

$$\sup_{(\mu,v)\in X_h} \frac{\langle \mathcal{G}'(\widehat{\lambda}, \widehat{u})(\gamma, w), (\mu, v)\rangle}{\|(\mu, v)\|_X} \gtrsim \|(\gamma, w)\|_X, \quad \forall (\gamma, w) \in X_h. \tag{23}$$

Proof For the first estimate (21), we just need to prove that the equation

$$\mathcal{G}'(\lambda, u)(\gamma, w) = (\tau, f) \tag{24}$$

is uniquely solvable in X for any $(\tau, f) \in X^*$. From (18), we obtain that (24) can be rewritten as

$$\begin{cases} \widehat{a}(\lambda, u; w, v) + \widehat{b}(u; v, \gamma) = (f, v), & \forall v \in V, \\ \widehat{b}(u; w, \mu) = \mu\tau, & \forall \mu \in \mathbb{R}. \end{cases}$$

For this saddle problem, the solvable condition is ([7, Theorem 1.1], II):
Firstly, the following variational problem

$$\widehat{a}(\lambda, u; w, v) = (f, v), \quad \forall v \in V_0 \tag{25}$$

is uniquely solvable with $V_0 := \{v \in V : \widehat{b}(u; v, \mu) = 0, \ \forall \mu \in \mathbb{R}\}$.
Secondly, $\widehat{b}(u; \cdot, \cdot)$ satisfies the inf-sup condition

$$\inf_{\mu\in\mathbb{R}} \sup_{v\in V} \frac{\widehat{b}(u; v, \mu)}{\|v\|_1|\mu|} \geq k_b \tag{26}$$

for some constant $k_b > 0$.

The well-posedness of (25) can be derived from (7) directly.

For the second condition (26), take $v = -\mu u$. Since $\|u\|_0 = 1$, there holds

$$\inf_{\mu\in\mathbb{R}} \sup_{v\in V} \frac{\widehat{b}(u; v, \mu)}{\|v\|_1|\mu|} \geq \inf_{\mu\in\mathbb{R}} \frac{\mu^2(u, u)}{\|u\|_1|\mu|^2} = \frac{1}{\|u\|_1} =: k_b.$$

This completes the proof of (21).

From (7), we can define a project operator $P_h : V \to V_h$ by

$$\widehat{a}(\lambda, u; w, v - P_h v) = 0, \quad \forall w \in V_h, \ v \in V. \tag{27}$$

There apparently holds

$$\|P_h v\|_1 \lesssim \|v\|_1, \quad \forall v \in V. \tag{28}$$

From the Aubin-Nitsche lemma, we have

$$\|v - P_h v\|_0 \lesssim \eta_a(V_h)\|v\|_1, \quad \forall v \in V. \tag{29}$$

So for any $(\gamma, w) \in X_h$, form (21) and (29), the following estimates hold

$$\begin{aligned}
\|(\gamma, w)\|_X &\lesssim \sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, v)\rangle}{\|(\mu, v)\|_X} \\
&= \sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, P_h v)\rangle + \langle \mathcal{G}'(\lambda, u)(\gamma, w), (0, v - P_h v)\rangle}{\|(\mu, v)\|_X} \\
&= \sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, P_h v)\rangle - \gamma(u, v - P_h v)}{\|(\mu, v)\|_X} \\
&\lesssim \sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, P_h v)\rangle + |\gamma|\|u\|_0\|v - P_h v\|_0}{\|(\mu, v)\|_X} \\
&\lesssim \sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, P_h v)\rangle + |\gamma|\eta_a(V_h)\|u\|_0\|v\|_1}{\|(\mu, v)\|_X} \\
&\lesssim \sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, P_h v)\rangle}{\|(\mu, v)\|_X} + \eta_a(V_h)\|(\gamma, w)\|_X.
\end{aligned} \tag{30}$$

When the mesh size h is small enough, combing (28) and (30) leads to

$$\begin{aligned}
\|(\gamma, w)\|_X &\lesssim \sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, P_h v)\rangle}{\|(\mu, v)\|_X} \\
&\lesssim \sup_{(\mu,v)\in X} \frac{\langle \mathcal{G}'(\lambda, u)(\gamma, w), (\mu, P_h v)\rangle}{\|(\mu, P_h v)\|_X}
\end{aligned}$$

$$\lesssim \sup_{(\mu,v)\in X_h} \frac{\langle \mathcal{G}'(\lambda,u)(\gamma,w),(\mu,v)\rangle}{\|(\mu,v)\|_X}.$$

Then we get the desired conclusion (22).

For the last inequality (23), we assume there exists a sufficiently small constant ε such that $\|(\widehat{\lambda}-\lambda,\widehat{u}-u)\|_X \le \varepsilon$. Then for any $(\gamma,w)\in X_h$

$$\begin{aligned}\|(\gamma,w)\|_X &\lesssim \sup_{(\mu,v)\in X_h} \frac{\langle \mathcal{G}'(\lambda,u)(\gamma,w),(\mu,v)\rangle}{\|(\mu,v)\|_X}\\ &\lesssim \sup_{(\mu,v)\in X_h} \frac{\langle \mathcal{G}'(\widehat{\lambda},\widehat{u})(\gamma,w),(\mu,v)\rangle + \varepsilon\|(\gamma,w)\|_X\|(\mu,v)\|_X}{\|(\mu,v)\|_X}.\end{aligned}$$

The desired result (23) then easily follows if ε is sufficiently small. □

Applying Newton iteration method to GPE leads to a linearized problem, the corresponding residual estimate can be derived from the following theorem.

Theorem 2 *For the nonlinear operator $\mathcal{G}$ and any $(\mu_h,v_h),(\mu,v)\in X$, we have*

$$\begin{aligned}\langle \mathcal{G}(\mu_h,v_h),(\sigma,\eta)\rangle &= \langle \mathcal{G}(\mu,v),(\sigma,\eta)\rangle + \langle \mathcal{G}'(\mu,v)(\mu_h-\mu,v_h-v),(\sigma,\eta)\rangle\\ &\quad + R\big((\mu,v),(\mu_h,v_h),(\sigma,\eta)\big), \qquad \forall(\sigma,\eta)\in X \end{aligned} \tag{31}$$

with $R\big((\mu,v),(\mu_h,v_h),(\sigma,\eta)\big)$ being the residual which can be estimated as follows:

$$\big|R\big((\mu,v),(\mu_h,v_h),(\sigma,\eta)\big)\big| \lesssim \|(\mu-\mu_h,v-v_h)\|_X\|(\mu-\mu_h,v-v_h)\|_0\|(\sigma,\eta)\|_X.$$

Proof Define

$$\varphi(t) = \langle \mathcal{G}((\mu,v)+t(\mu_h-\mu,v_h-v)),(\sigma,\eta)\rangle. \tag{32}$$

Then the derivative of φ with respect to t can be derived trivially as follows

$$\begin{aligned}\varphi'(t) &= (\nabla(v_h-v),\nabla\eta) + (W(v_h-v),\eta) + 3\big(\zeta(v+t(v_h-v))^2(v_h-v),\eta\big)\\ &\quad - (\mu_h-\mu)(v+t(v_h-v),\eta) - (\mu+t(\mu_h-\mu))(v_h-v,\eta)\\ &\quad - \sigma(v+t(v_h-v),v_h-v)\\ &= \langle \mathcal{G}'((\mu,v)+t(\mu_h-\mu,v_h-v))(\mu_h-\mu,v_h-v),(\sigma,\eta)\rangle\end{aligned}$$

and

$$\begin{aligned}\varphi''(t) &= -2(\mu_h-\mu)(v_h-v,\eta) - \sigma(v_h-v,v_h-v)\\ &\quad + 6(\zeta(v+t(v_h-v))(v_h-v)^2,\eta).\end{aligned} \tag{33}$$

Denote $\xi = v+t(v_h-v)$ and from the imbedding theorem, we have

$$\|\xi\|_{0,6} \lesssim \|\xi\|_1 \lesssim \|v\|_1 + \|v_h\|_1.$$

For the last term of (33),

$$\begin{aligned}|(\xi(v_h - v)^2, \eta)| &\lesssim \int_\Omega |\xi|(v_h - v)^2|\eta| dx \\ &\lesssim \|\xi\|_{0,6}\|v_h - v\|_0\|v_h - v\|_{0,6}\|\eta\|_{0,6} \\ &\lesssim \|\xi\|_1\|v_h - v\|_1\|v_h - v\|_0\|\eta\|_1. \end{aligned} \tag{34}$$

Thus, (31) can be derived from the following Taylor expansion

$$\varphi(1) = \varphi(0) + \varphi'(0) + \int_0^1 \varphi''(t)(1-t)dt. \tag{35}$$

Due to (33)–(35), the residual R satisfies

$$\left|R\big((\mu, v), (\mu_h, v_h), (\sigma, \eta)\big)\right| \lesssim \|(\mu - \mu_h, v - v_h)\|_X\|(\mu - \mu_h, v - v_h)\|_0\|(\sigma, \eta)\|_X.$$

Then we complete the proof. □

4 Multigrid algorithm based on Newton iteration method

In this section, we propose a multigrid scheme based on Newton iteration method. In this algorithm, we only need to solve a linearized mixed problem on each refined finite element space.

4.1 One Newton iteration step

In order to design the multigrid method, we first introduce an one Newton iteration step in this subsection. Assume we have obtained an eigenpair approximation $(\lambda^{h_k}, u^{h_k}) \in \mathbb{R} \times V_{h_k}$, a type of iteration step will be introduced to derive an eigenpair $(\lambda^{h_{k+1}}, u^{h_{k+1}}) \in \mathbb{R} \times V_{h_{k+1}}$ with a better accuracy. In this paper, we denote by (λ_{h_k}, u_{h_k}) the standard finite element solution of (4).

Theorem 3 *After implementing Algorithm 1, the resultant eigenpair approximation* $(\lambda^{h_{k+1}}, u^{h_{k+1}})$ *has the following error estimate*

$$\begin{aligned}&\|(\lambda^{h_{k+1}} - \lambda_{h_{k+1}}, u^{h_{k+1}} - u_{h_{k+1}})\|_X \\ &\lesssim \eta_a(V_{h_{k+1}})\delta_{h_{k+1}}(u) + \delta_{h_k}(u)\|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_X \\ &\quad + \|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_X\|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_0. \end{aligned} \tag{37}$$

Proof For the standard finite element solution $(\lambda_{h_{k+1}}, u_{h_{k+1}})$, we have

$$\langle \mathcal{G}(\lambda_{h_{k+1}}, u_{h_{k+1}}), (\mu, v_{h_{k+1}})\rangle = 0, \quad \forall (\mu, v_{h_{k+1}}) \in X_{h_{k+1}}. \tag{38}$$

Algorithm 1: One Newton Iteration Step

1. Define the linearized mixed variational equation on the finite element space $X_{h_{k+1}}$ as follows: Find $(\widehat{\lambda}^{h_{k+1}}, \widehat{u}^{h_{k+1}}) \in X_{h_{k+1}}$ such that for all $(\mu, v_{h_{k+1}}) \in X_{h_{k+1}}$

$$\begin{cases} \widehat{a}(\lambda^{h_k}, u^{h_k}; \widehat{u}^{h_{k+1}}, v_{h_{k+1}}) + \widehat{b}(u^{h_k}; v_{h_{k+1}}, \widehat{\lambda}^{h_{k+1}}) = (f, v_{h_{k+1}}), \\ \widehat{b}(u^{h_k}; \widehat{u}^{h_{k+1}}, \mu) = (g, \mu), \end{cases} \tag{36}$$

   where $f = 2\zeta(u^{h_k})^3 - \lambda^{h_k} u^{h_k}$, $g = -(1 + (u^{h_k}, u^{h_k}))/2$.
2. Solve equation (36) to obtain an eigenpair approximation $(\lambda^{h_{k+1}}, u^{h_{k+1}})$ satisfying $\|(\lambda^{h_{k+1}} - \widehat{\lambda}^{h_{k+1}}, u^{h_{k+1}} - \widehat{u}^{h_{k+1}})\|_X \lesssim \eta_a(V_{h_{k+1}})\delta_{h_{k+1}}(u)$.

In order to simplify the notation and summarize the above two steps, we define

$$(\lambda^{h_{k+1}}, u^{h_{k+1}}) = Newton\_Iteration\_Step(\lambda^{h_k}, u^{h_k}, V_{h_{k+1}}).$$

Together with (31) and (36) in Algorithm 1, there holds

$$\begin{aligned} &\langle \mathcal{G}'(\lambda^{h_k}, u^{h_k})(\lambda_{h_{k+1}} - \widehat{\lambda}^{h_{k+1}}, u_{h_{k+1}} - \widehat{u}^{h_{k+1}}), (\mu, v_{h_{k+1}})\rangle \\ &\quad = \langle \mathcal{G}(\lambda^{h_k}, u^{h_k}), (\mu, v_{h_{k+1}})\rangle \\ &\qquad + \langle \mathcal{G}'(\lambda^{h_k}, u^{h_k})(\lambda_{h_{k+1}} - \lambda^{h_k}, u_{h_{k+1}} - u^{h_k}), (\mu, v_{h_{k+1}})\rangle \\ &\quad = \langle \mathcal{G}(\lambda^{h_k}, u^{h_k}), (\mu, v_{h_{k+1}})\rangle - \langle \mathcal{G}(\lambda_{h_{k+1}}, u_{h_{k+1}}), (\mu, v_{h_{k+1}})\rangle \\ &\qquad + \langle \mathcal{G}'(\lambda^{h_k}, u^{h_k})(\lambda_{h_{k+1}} - \lambda^{h_k}, u_{h_{k+1}} - u^{h_k}), (\mu, v_{h_{k+1}})\rangle \\ &\quad = -R\big((\lambda^{h_k}, u^{h_k}), (\lambda_{h_{k+1}}, u_{h_{k+1}}), (\mu, v_{h_{k+1}})\big). \end{aligned} \tag{39}$$

Using (23), Theorem 2 and (39), we derive

$$\begin{aligned} &\|(\lambda_{h_{k+1}} - \widehat{\lambda}^{h_{k+1}}, u_{h_{k+1}} - \widehat{u}^{h_{k+1}})\|_X \\ &\lesssim \|(\lambda_{h_{k+1}} - \lambda^{h_k}, u_{h_{k+1}} - u^{h_k})\|_X \|(\lambda_{h_{k+1}} - \lambda^{h_k}, u_{h_{k+1}} - u^{h_k})\|_0 \\ &\lesssim \big(\|(\lambda_{h_{k+1}} - \lambda_{h_k}, u_{h_{k+1}} - u_{h_k})\|_X + \|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_X\big) \\ &\quad \big(\|(\lambda_{h_{k+1}} - \lambda_{h_k}, u_{h_{k+1}} - u_{h_k})\|_0 + \|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_0\big) \\ &\lesssim \eta_a(V_{h_k})\delta_{h_k}^2(u) + \delta_{h_k}(u)\|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_X \\ &\quad + \|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_X \|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_0. \end{aligned} \tag{40}$$

Since

$$\|(\lambda^{h_{k+1}} - \widehat{\lambda}^{h_{k+1}}, u^{h_{k+1}} - \widehat{u}^{h_{k+1}})\|_X \lesssim \eta_a(V_{h_{k+1}})\delta_{h_{k+1}}(u),$$

we arrive at

$$\begin{aligned} &\|(\lambda^{h_{k+1}} - \lambda_{h_{k+1}}, u^{h_{k+1}} - u_{h_{k+1}})\|_X \\ &\quad \lesssim \eta_a(V_{h_{k+1}})\delta_{h_{k+1}}(u) + \delta_{h_k}(u)\|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_X \end{aligned}$$

$$+ \|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_X \|(\lambda_{h_k} - \lambda^{h_k}, u_{h_k} - u^{h_k})\|_0.$$

This completes the proof. □

4.2 Multilevel correction method

In order to do multigrid iteration, we define a sequence of triangulations $\mathcal{T}_{h_k}$, in which $\mathcal{T}_{h_{k+1}}$ is produced from $\mathcal{T}_{h_k}$ via a regular refinement (produce β^d congruent elements) such that

$$h_k \approx \frac{1}{\beta} h_{k-1}, \tag{41}$$

where the constant β denotes the refinement index and larger than 1 (always equals 2). Based on the mesh sequence, we construct a series of linear finite element spaces satisfying

$$V_{h_1} \subset V_{h_2} \subset \cdots \subset V_{h_n} \subset V \tag{42}$$

and assume the following relations of approximation errors hold

$$\eta_a(V_{h_k}) \approx \frac{1}{\beta} \eta_a(V_{h_{k-1}}), \quad \delta_{h_k}(u) \approx \frac{1}{\beta} \delta_{h_{k-1}}(u), \quad k = 1, 2, \ldots, n. \tag{43}$$

Obviously, the following relationship is also valid

$$X_{h_1} \subset X_{h_2} \subset \cdots \subset X_{h_n} \subset X. \tag{44}$$

The multigrid method based on one Newton iteration step is defined by Algorithm 2.

Algorithm 2: Multigrid Algorithm

1. Construct a series of nested finite element spaces $V_{h_1}, V_{h_2}, \ldots, V_{h_n}$ such that (42) and (43) hold.
2. Solve the GPE on the initial finite element space X_{h_1}: Find $(\lambda_{h_1}, u_{h_1}) \in X_{h_1}$ such that

$$(\nabla u_{h_1}, \nabla v_{h_1}) + (W u_{h_1}, v_{h_1}) + (\zeta (u_{h_1})^3, v_{h_1}) = \lambda_{h_1} (u_{h_1}, v_{h_1}), \quad \forall v \in V_{h_1}.$$

   Using iteration method to solve this nonlinear eigenvalue problem and obtain $(\lambda^{h_1}, u^{h_1}) \in X_{h_1}$ with error estimate $\|(\lambda_{h_1} - \lambda^{h_1}, u_{h_1} - u^{h_1})\|_X \lesssim \eta_a(V_{h_1}) \delta_{h_1}(u)$.
3. Do $k = 1, \ldots, n-1$
   Obtain a new eigenpair approximation $(\lambda^{h_{k+1}}, u^{h_{k+1}})$ by a Newton iteration step

$$(\lambda^{h_{k+1}}, u^{h_{k+1}}) = Newton\_Iteration\_Step(\lambda^{h_k}, u^{h_k}, V_{h_{k+1}}).$$

   End Do.

Theorem 4 *Assume the initial mesh size h_1 is sufficiently small, after implementing Algorithm 2, the resultant eigenpair approximation (λ^{h_n}, u^{h_n}) has the following error estimate*

$$\|(\lambda_{h_n} - \lambda^{h_n}, u_{h_n} - u^{h_n})\|_X \lesssim \eta_a(V_{h_n})\delta_{h_n}(u). \tag{45}$$

Proof We use mathematical induction to give the proof. At first, from the second step of Algorithm 2, we know that (45) holds for the initial finite element space X_{h_1}. Then, assume that (45) is true for the space $V_{h_{n-1}}$, i.e.

$$\|(\lambda_{h_{n-1}} - \lambda^{h_{n-1}}, u_{h_{n-1}} - u^{h_{n-1}})\|_X \lesssim \eta_a(V_{h_{n-1}})\delta_{h_{n-1}}(u).$$

Now, we consider the error estimates in the space V_{h_n}. Using Theorem 3 and our assumption, we have

$$\begin{aligned}
&\|(\lambda_{h_n} - \lambda^{h_n}, u_{h_n} - u^{h_n})\|_X \\
&\quad\lesssim \eta_a(V_{h_n})\delta_{h_n}(u) + \delta_{h_{n-1}}(u)\|(\lambda_{h_{n-1}} - \lambda^{h_{n-1}}, u_{h_{n-1}} - u^{h_{n-1}})\|_X \\
&\qquad + \|(\lambda_{h_{n-1}} - \lambda^{h_{n-1}}, u_{h_{n-1}} - u^{h_{n-1}})\|_X\|(\lambda_{h_{n-1}} - \lambda^{h_{n-1}}, u_{h_{n-1}} - u^{h_{n-1}})\|_0 \\
&\quad\lesssim \eta_a(V_{h_n})\delta_{h_n}(u),
\end{aligned}$$

which means that (45) is also valid for the space V_{h_n}. Then, we complete the proof. □

At last, we give the error estimates for the final eigenpair approximation (λ^{h_n}, u^{h_n}) which is obtained by Algorithm 2.

Theorem 5 *For Algorithm 2, under the conditions of Thoerem 4, we have*

$$\|u - u^{h_n}\|_1 \lesssim \delta_{h_n}(u), \tag{46}$$

$$\|u - u^{h_n}\|_0 \lesssim \eta_a(V_{h_n})\delta_{h_n}(u), \tag{47}$$

$$|\lambda - \lambda^{h_n}| \lesssim \eta_a(V_{h_n})\delta_{h_n}(u). \tag{48}$$

Proof From Lemma 2 and Theorem 4, we have

$$\begin{aligned}
&\|(\lambda - \lambda^{h_n}, u - u^{h_n})\|_X \\
&\quad\le \|(\lambda - \lambda_{h_n}, u - u_{h_n})\|_X + \|(\lambda_{h_n} - \lambda^{h_n}, u_{h_n} - u^{h_n})\|_X \\
&\quad\lesssim \delta_{h_n}(u),
\end{aligned}$$

which means that (46) holds. Similarly, there holds

$$\|(\lambda - \lambda^{h_n}, u - u^{h_n})\|_0 \lesssim \eta_a(V_{h_n})\delta_{h_n}(u).$$

Then, we get (47) and (48) immediately, and the proof is completed. □

Remark 1 For the discrete linear system (36) involved in each level of Algorithm 1, we can adopt the multigrid method to solve it efficiently (see e.g., [6,29]).

5 Work estimate of multigrid algorithm

In this section, the computational work of Algorithm 2 is presented to show the efficiency of this multigrid scheme. Denote the dimension of finite element space V_{h_k} by N_k. Then we have

$$N_k \approx \beta^{d(k-n)} N_n, \quad k = 1, 2, \ldots, n.$$

Theorem 6 *Assume the work of GPE problem in the initial finite element space V_{h_1} is $\mathcal{O}(M_{h_1})$ and that of the linear boundary value problem in each level V_{h_k} is $\mathcal{O}(N_k)$ for $k = 1, 2, \ldots, n$. Then the work involved in the multigrid method is $\mathcal{O}(N_n + M_{h_1})$. Furthermore, the complexity can be $\mathcal{O}(N_n)$ provided $M_{h_1} \leq N_n$.*

Proof Denote the work in the k-th finite element space V_{h_k} by W_k and the total work by W. Then

$$\begin{aligned} W &= \sum_{k=1}^{n} W_k = \mathcal{O}\big(M_{h_1} + \sum_{k=2}^{n} N_k\big) = \mathcal{O}\big(M_{h_1} + \sum_{k=2}^{n} \beta^{d(k-n)} N_n\big) \\ &= \mathcal{O}(M_{h_1} + N_n). \end{aligned}$$

Then we derive the desired result and $W = \mathcal{O}(N_n)$ when $M_{h_1} \leq N_n$. □

6 Numerical results

In this section, three numerical examples are presented to illustrate the efficiency of the multigrid scheme proposed in this paper. Since the aim here is to show the efficiency of the proposed scheme, we choose the computing domain as the unit square or cube without loss of generality. Here, we use the multigrid method to solve the linear system (36). The distributive Gauss-Seidel (DGS) is adopted as the smoothers [6,14]. The linear problem (36) is solved by V-cycle multigrid method with two pre-smoothing and post-smoothing steps. In step 2 of Algorithm 2, we need to solve the nonlinear eigenvalue problem in V_{h_1}. The self-consistent method is adopted and package ARPACK is called here for the linear eigenvalue problems involved in each self-consistent iteration step. In this paper, all schemes are running on the same machine PowerEdge R720 with the Linux system. The machine is equipped with Intel Xeon E5-2620 (2.00GHz) CPU with 72G memory.

6.1 Example 1

In the first example, we use Algorithm 2 to solve the following GPE on the unit square: Find (λ, u) such that

$$\begin{cases} -\triangle u + Wu + \zeta |u|^2 u = \lambda u, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, \\ \int_\Omega u^2 d\Omega = 1, \end{cases} \tag{49}$$

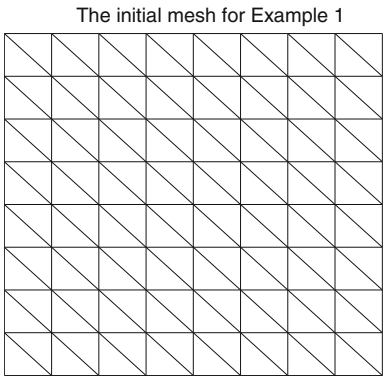

Fig. 1 The initial mesh for Example 1

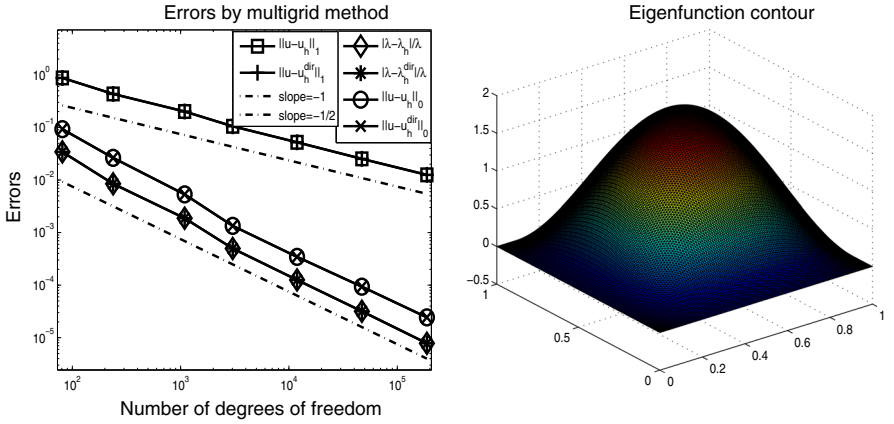

Fig. 2 Left: The errors of the multigrid method for the ground state solution of GPE, where λ_h and u_h denote the numerical solutions of Algorithm 2, λ_h^{dir} and u_h^{dir} denote the numerical solutions of the direct finite element method. Right: The contour of the ground state solution of Algorithm 2 for Example 1

where $\Omega = [0, 1]^2$, $W = x_1^2 + x_2^2$ and $\zeta = 1$.

Figure 1 shows the initial mesh for (49). The sequence of finite element spaces is constructed by linear element on a series of meshes produced by regular refinement with $\beta = 2$ (producing β^2 congruent subelements). Since the exact eigenpair is unknown, we choose an adequately accurate approximation defined on a further refined mesh as the exact solution for our numerical tests. In order to exhibit the accuracy of the approximate solution derived by Algorithm 2, we also solve (49) directly by the finite element method for comparison.

The corresponding numerical results and the eigenfunction contour are depicted in Fig. 2. From Fig. 2, we can find that Algorithm 2 is able to obtain the optimal approximations, which is in consistent with Theorem 5. Besides, this figure also shows that Algorithm 2 can achieve the same optimal error estimates as the direct finite element method for (49).

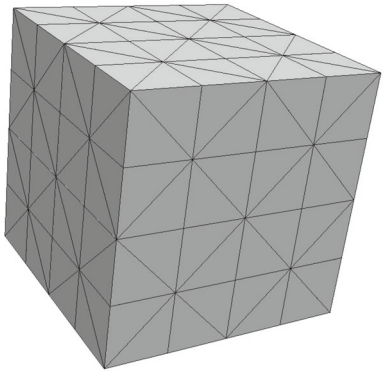

Fig. 3 The initial mesh for Example 2

6.2 Example 2

In the second example, we use Algorithm 2 to solve the following GPE on a three dimensional domain: Find (λ, u) such that

$$\begin{cases} -\triangle u + Wu + \zeta |u|^2 u = \lambda u, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, \\ \int_\Omega u^2 d\Omega = 1, \end{cases} \tag{50}$$

where Ω denotes the unit cube $[0, 1]^3$, $W = x_1^2 + x_2^2 + x_3^2$ and $\zeta = 1$.

Figure 3 shows the initial mesh. The sequence of finite element spaces is constructed by linear element on a series of meshes produced by regular refinement with $\beta = 2$ (connecting the midpoint of each edge). Since the exact solution is also unknown, an adequately accurate approximation defined on a further refined mesh is chosen as the exact solution to investigate the convergence behavior. In order to exhibit the accuracy of the approximate solution derived by Algorithm 2, we also solve (50) directly by the finite element method in the finest mesh, where the package ARPACK with CG iteration is called.

The numerical results by Algorithm 2 and the direct finite element method are depicted in Fig. 4 (left). These numerical results show that Algorithm 2 is able to obtain the optimal approximations as the direct finite element method, which is in consistent with Theorem 5. In order to show the efficiency of Algorithm 2, we compare CPU time (in seconds) between Algorithm 2 and the direct finite element method in finest mesh. The corresponding results are presented in Fig. 4 (right) and Table 1, which imply the efficiency and linear scale complexity of Algorithm 2, and agree with Theorem 6. From Table 1, we also find that Algorithm 2 has higher efficiency than the direct finite element method.

6.3 Example 3

In the third example, we consider the GPE (50) on the unit domain $\Omega = [0, 1]^3$ with the coefficient $W = x_1^2 + 2x_2^2 + 4x_3^2$ and $\zeta = 100$. Figure 5 gives the initial mesh for

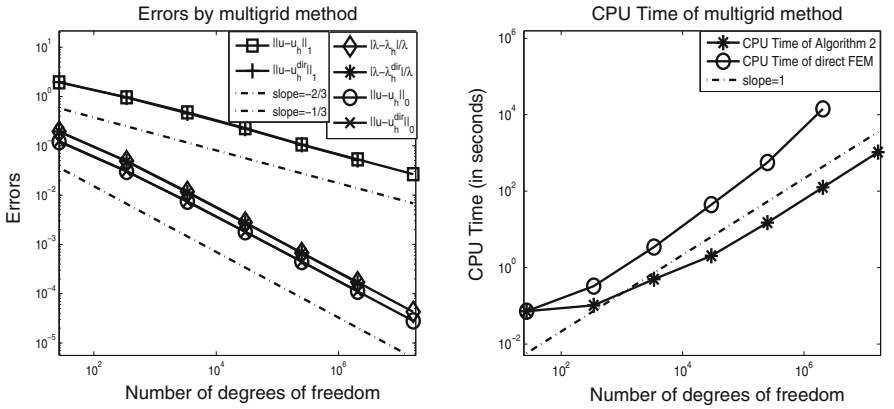

Fig. 4 Left: The errors of the multigrid method for the ground state solution of GPE, where λ_h and u_h denote the numerical solutions of Algorithm 2, λ_h^{dir} and u_h^{dir} denote the numerical solutions of the direct finite element method. Right: CPU Time of Algorithm 2 for Example 2

Table 1 The CPU time of Algorithm 2 and the direct finite element method for Example 2. The symbol "−" means the computer runs out of memory

Number of levels	Number of degrees of freedom	Time of Algorithm 2	Time of direct FEM
1	27	0.0723	0.0723
2	343	0.1035	0.3280
3	3375	0.4989	3.4613
4	29791	2.0394	44.5336
5	250047	15.0021	564.0327
6	2048383	125.7923	14180.5070
7	16581375	1048.6247	–

this example. The numerical results are presented in Fig. 6 and Table 2, which also show the convergence behavior and efficiency of Algorithm 2.

Since larger ζ leads to stronger nonlinearity, the initial mesh in this example is chosen finer than the second example with $\zeta = 1$. The stronger nonlinearity will also lead more self-consistent iterations which means solving the nonlinear eigenvalue problem in the initial mesh needs more CPU time. This fact can be found from Tables 1 and 2. In our multigrid scheme (Algorithm 2), only one linear problem is required to be solved on each refined mesh. Thus, even solving nonlinear eigenvalue problem on the coarse mesh needs more CPU time for $\zeta = 100$, the total CPU time becomes almost the same as that for $\zeta = 1$ when the discretization scale is large enough.

7 Concluding remarks

In this paper, we propose a type of multigrid method for GPE problems based on Newton iteration scheme. Different from the classical nonlinear eigensolver for GPE

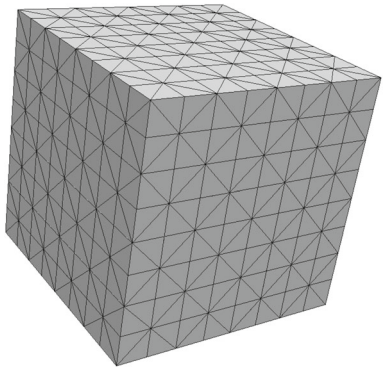

Fig. 5 The initial mesh for Example 3

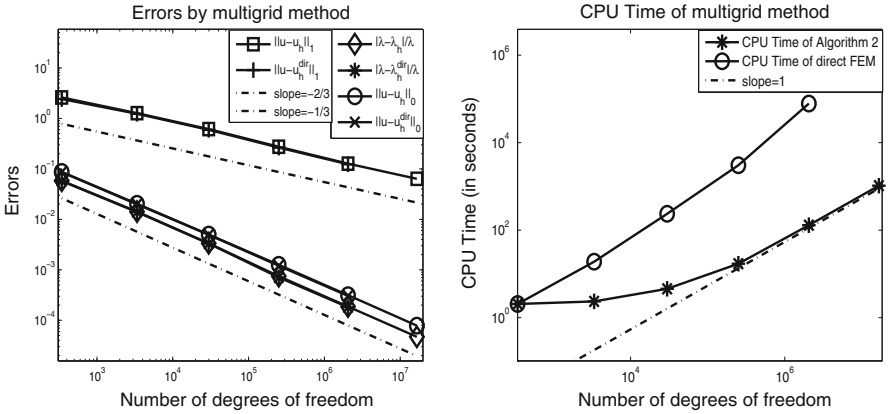

Fig. 6 Left: The errors of the multigrid method for the ground state solution of GPE, where λ_h and u_h denote the numerical solutions of Algorithm 2, λ_h^{dir} and u_h^{dir} denote the numerical solutions of the direct finite element method. Right: CPU Time of Algorithm 2 for Example 3

Table 2 The CPU time of Algorithm 2 and the direct finite element method for Example 3. The symbol "$-$" means the computer runs out of memory

Number of levels	Number of degrees of freedom	Time of Algorithm 2	Time of direct FEM
1	343	2.0532	2.0532
2	3375	2.3456	19.0372
3	29791	4.5544	236.0440
4	250047	17.0574	3045.7766
5	2048383	129.6357	77990.3764
6	16581375	1035.5986	–

problems, the proposed method transforms the nonlinear eigenvalue problem solving to a series of linear boundary value problem solving and an nonlinear eigenvalue problem solving in the coarsest finite element space. The high efficiency of linear boundary value problems solving can improve the overall efficiency of the simulation for BEC. The idea proposed here can also be extended to other nonlinear eigenvalue problems, such as Kohn-Sham equation, which always arises from the electronic structure simulation.

As the classical multigrid method, our algorithm runs on a nested mesh sequence. If some complicated domains are given such that we can not construct a nested mesh sequence, then we need to use the special prolongation and restriction operators designed for multigrid method on non-nested mesh sequence, see e.g. [31]. In this case, our algorithm can still be performed but the theoretical analysis presented in this paper needs to be done the corresponding modification.

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