Superconvergence of bi-\(k\)-Lagrange elements for eigenvalue problems

Z.-C. Li\(^a,b\), C.-S. Chien\(^c,*,1\), H.-T. Huang\(^d\), B.-W. Jeng\(^e\)

\(^a\) Department of Applied Mathematics, and Department of Computer Science and Engineering, National Sun Yat-sen University, Kaohsiung 804, Taiwan
\(^b\) Department of Applied Mathematics, Chung-Hua University, Sinchu 300, Taiwan
\(^c\) Department of Computer Science and Information Engineering, Ching Yun University, Jungli 320, Taiwan
\(^d\) Department of Applied Mathematics, I-Shou University, Kaohsiung County 840, Taiwan
\(^e\) Department of Mathematics Education, National Taichung University, Taichung 403, Taiwan

\(^*\) Corresponding author.

E-mail addresses: zcli@math.nsysu.edu.tw (Z.-C. Li), cschien@amath.nchu.edu.tw (C.-S. Chien).

\(^1\) Supported by the National Science Council of ROC (Taiwan) through Project NSC 95-2115-M231-001-MY3.

Abstract

We study superconvergence of bi-\(k\)-Lagrange elements for parameter-dependent problems where \(k \geq 2\). We show that the superconvergence rate of the bi-\(k\)-Lagrange elements is two orders higher than that of the \(k\)th-order Lagrange elements. This is a significant improvement of the previous results [C.-S. Chien, H.T. Huang, B.-W. Jeng, Z.C. Li, Superconvergence of FEMS and numerical continuation for parameter-dependent problems with folds, Int. J. Bifurcation Chaos 18 (2008) 1321–1336], which is only one order (or a half order) higher than that of the latter. Next, we apply the bi-\(k\)-Lagrange elements to the computations of energy levels and wave functions of two-dimensional (2D) Bose–Einstein condensates (BEC), and BEC in a periodic potential. Sample numerical results are reported.

© 2009 Elsevier B.V. All rights reserved.

1. Introduction

During the past years many encouraging results on superconvergence have been obtained for the Poisson equation \([1–4]\)

\[-\Delta \mathcal{A} \mathcal{V} = g (x, y) \quad \text{in } \mathcal{A},\]

\[u = 0 \quad \text{on } \partial \mathcal{A},\]

(1.1)

where \(\mathcal{A} \subseteq \mathbb{R}^2\) is a polygon, and \(g\) a smooth function of \((x, y)\). By superconvergence we mean that the convergence rate of the \(k\)th-order elements is higher than the optimal convergence rate \(O(h^k)\). In [1] we studied the Adini elements for (1.1). We showed that the superconvergence rate of the third order Adini elements is a half order higher than \(O(h^3)\), and that the superconvergence rate of the \(k\)th-order Lagrange elements is one order higher than \(O(h^k)\). In this paper, we will study superconvergence of the bi-\(k\)-Lagrange elements for (1.1), where \(k \geq 2\). Next, we will apply the bi-\(k\)-Lagrange elements combined with numerical continuation methods to investigate numerical solutions of parameter-dependent problems of the form

\[F(\lambda, \mathcal{V}) = -\Delta \mathcal{V} - \lambda f (\mathcal{V}) = 0 \quad \text{in } \mathcal{A},\]

\[\mathcal{V} = 0 \quad \text{on } \partial \mathcal{A},\]

(1.2)

where \(f\) is a smooth function of \(\mathcal{V}\) which satisfies certain smooth conditions. An interesting example of (1.2) is the stationary state nonlinear Schrödinger equation (NLS) or the Gross–Pitaevskii equation (GPE) \([5,6]\).

Let \(h\) be the uniform length of edges of rectangular elements for the domain \(\mathcal{A}\). Let \(\mathcal{V}\) be the exact solution of (1.1), and \(\mathcal{V}_I\) the finite element method (FEM) interpolant of \(\mathcal{V}\). By treating \(\mathcal{V}_I\) as the point-line-area interpolant \([4]\), we prove that the superconvergence rate of the bi-\(k\)-Lagrange element approximations is two orders higher than the optimal convergence rate \(O(h^k)\), which is a significant improvement of the previous result [1].
One of our aims here is to study energy levels and wave functions of Bose–Einstein condensates (BEC) [7–9] which is governed by the NLS or the GPE [5,6]

\[ i \frac{\partial}{\partial t} \Psi(x,t) = -\Delta \Psi + V(x)\Psi + \mu |\Psi|^2 \Psi, \quad t > 0, \quad x = (x, y) \in \Omega, \]

\[ \Psi(x,t) = 0, \quad x \in \partial \Omega, \quad t \geq 0, \tag{1.3} \]

where \( \Psi = \Psi(x,t) \) is the macroscopic wave function of the BEC, \( V(x) = \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) \) the magnetic trapping potential with \( \gamma_x \) and \( \gamma_y \) the trap frequencies in the x- and y-coordinate, the constant \( \mu \) can be positive or negative, and \( \Omega \subset \mathbb{R}^2 \) a bounded domain with piecewise smooth boundary \( \partial \Omega \). Eq. (1.3) can be easily generalized to M-component NLS, \( M \geq 2 \). An important invariant of the NLS is the mass conservation constraint, or the normalization of the wave function

\[ \int_{\Omega} |\Psi(x,t)|^2 \, dx = 1, \quad t \geq 0, \tag{1.4} \]

which means that the total probability of finding the particle anywhere in \( \Omega \) must be 1.

Next, we will study energy levels and wave functions of BEC in a periodic potential which is governed by

\[ i \frac{\partial \Psi}{\partial t} = -\Delta \Psi + V(x) + a_1 \sin^2 \left( \frac{\pi x}{d_1} \right) + a_2 \sin^2 \left( \frac{\pi y}{d_2} \right) \Psi + \mu |\Psi|^2 \Psi, \quad x \in \Omega, \]

\[ \Psi(x,t) = 0, \quad x \in \partial \Omega, \quad t \geq 0, \tag{1.5} \]

where constants \( a_1 \) and \( a_2 \) denote the depths of the potential in the x- and y-coordinates and are defined as

\[ a_j = \left( \frac{2}{3} \right) \hbar \Gamma \left( \frac{1}{I_j} \right), \quad j = 1, 2, \]

with \( I \) the intensity of one laser beam, \( I_j \) the saturation intensity of the atomic/molecular resonance line, \( \Gamma \) the decay rate of the first excited-state, \( \gamma \) the detuning of the lattice beams from the atomic resonance [10], and \( d_j \) the distance of neighbor wells.

Recently, some variants of the imaginary time evolution method (ITEM) have been proposed for computing the ground-state solution of (1.3). For instance, García-Ripoll and Pérez-García [11] exploited a version of the ITEM namely, ITS, to minimize

\[ E(\Psi) = \iint_{\Omega} \left[ \frac{1}{2} |\nabla \Psi(x,t)|^2 + V(x) |\Psi(x,t)|^2 + \frac{\mu}{2} |\Psi(x,t)|^4 \right] \, dx, \tag{1.6} \]

using the Sobolev gradient of the energy functional as the preconditioner. Analogously, a version of the ITEM, namely, the continuous normalized gradient flow (CNGF) was also exploited in [12,13]. However, the convergence rate of the ITEM can be very slow [14], and in fact, it may diverge [15] if we replace the trapping potential \( V(x) \) in (1.3) by trigonometric functions. Recently, Yang and Lakoba [14] proposed accelerated ITEMs, called AITEM and AITEM with amplitude normalization (AITEM (A.N.)). Both AITEM and AITEM (A.N.) have significantly improved the convergence rate of the ITEM for this case.

To find energy levels and wave functions of the BEC, we substitute the formula

\[ \Psi(x,t) = e^{-i\lambda t} u(x) \tag{1.7} \]

into (1.3) and (1.5), and obtain the associated nonlinear eigenvalue problems

\[ -\Delta u(x) - \lambda u(x) + V(x) u(x) + \mu |u(x)|^2 u(x) = 0, \quad x \in \Omega, \]

\[ u(x) = 0, \quad x \in \partial \Omega, \tag{1.8} \]

and

\[ -\Delta u(x) - \lambda u(x) + \left[ V(x) + a_1 \sin^2 \left( \frac{\pi x}{d_1} \right) + a_2 \sin^2 \left( \frac{\pi y}{d_2} \right) \right] u(x) + \mu |u(x)|^2 u(x) = 0, \quad x \in \Omega, \]

\[ u(x) = 0, \quad x \in \partial \Omega, \tag{1.9} \]

respectively, where \( \lambda \) is the chemical potential of the condensate, and \( u(x) \) the stationary state real wave function which is independent of \( t \). In numerical continuation methods [15,16] we use modes of the linear counterparts, namely, the Schrödinger eigenvalue problems (SEP) corresponding to (1.8) and (1.9) to approximate modes of the nonlinear problems, where \( \lambda \) is treated as the continuation parameter. Note that eigenvalues of the SEP are just bifurcation points of the NLS on the trivial solution curve \( \{ (\lambda, u) = (\lambda, 0) \mid \lambda \in \mathbb{R}^+ \} \). We use predictor–corrector continuation methods to trace a solution curves of the NLS branching from a bifurcation point of the NLS. We stop the curve-tracking whenever the mass conservation constraint

\[ \iint_{\Omega} |u^*(x)|^2 \, dx = 1 \tag{1.10} \]

is satisfied, where \( (\lambda^*, u^*) \) is regarded as a target point on the solution curve.

This paper is organized as follows. In Section 2 we study superconvergence of bi-k-Lagrange element approximations for parameter-dependent problems, and in particular, for (1.8) and (1.9). A continuation algorithm using biquadratic Lagrange element approximations is described in Section 3 for curve-tracking. In Section 4 we discuss efficient implementations of continuation algorithms for curve-tracking. We also briefly discuss the performance of efficient continuation algorithms we have proposed for computing energy levels of BEC. Our numerical results are reported in Section 5. Finally, some concluding remarks are given in Section 6.
2. Superconvergence of the bi-$k$-Lagrange elements

Let $u$ and $u_I$ be defined as in Section 1. Let $v_k = \frac{\partial u}{\partial x}$, and so on. Denote $H^1_0(S) = \{v | v, v_y \in L^2(S) \text{ and } v|_{\partial S} = 0\}$. The superconvergence rate for the $k$th-order elements can be expressed in terms of

$$\frac{\left|\int_S \nabla (u_I - u_h) \cdot \nabla w\right|}{\|w\|_{1,5}} \leq C h^{k+q} \|u\|_{k+2.5}, \quad \forall w \in H^1_0(S),$$

where $u_h \in V^h_0 \subset H^1(S)$ is the FEM solution of (1.1). The subspace $V^h_0$ will be specified later. It was shown in [1] that $q = 0.5$ and $q = 1$ were obtained for (1.2) for the Adini elements and the $k$th-order Lagrange FEM, respectively, on the rectangles $\square_{ij}$. In this paper, we prove that $q = 2$ for the bi-$k$-Lagrange elements using the point-line-area elements. To prove (2.1), we need the following strong monotonicity [1] of (1.2),

$$a(u_h, u_I - u_h) - a(u_I, u_I - u_h) \geq c_0 \|u_I - u_h\|_{1,5}^2,$$

where $c_0$ is a positive constant independent of $h$, and

$$a(u, v) = \int_S \nabla u \cdot \nabla v - \lambda \int f(u)v.$$

Note that for $k = 1$, the bilinear elements have the superconvergence

$$\frac{\left|\int_S \nabla (u_I - u_h) \cdot \nabla w\right|}{\|w\|_{1,5}} \leq C h^2 \|u\|_{3,5}, \quad \forall w \in H^1_0(S),$$

which is one order higher than the optimal rate $O(h)$. Then the superconvergence rate $O(h^2)$ for (1.2) can be obtained directly from [1]. Hence the case $k = 1$ is not discussed in this paper. We will show that a higher superconvergence with $q = 2$ in (2.1) can be obtained for (1.2).

Denote the sets of polynomials of order less than or equal to $k$ by the $k$th-order polynomial $P_k$ in 1D and the bi-$k$th-order polynomial $Q_k$ in 2D, and

$$p_k(x) = \sum_{i=0}^k b_i x^i \in P_k,$$

$$q_k(x, y) = \sum_{i,j=0}^k a_{ij} x^i y^j \in Q_k,$$

where $b_i$ and $a_{ij}$ are constants. Let $S$ be divided into small uniform rectangles $\square_{ij}$, i.e., $S = \bigcup_{ij} \square_{ij}$. We define the following bi-$k$ interpolant $u_I$ of $u$ by means of the point-line-area elements on $e = \square_{ij}$ [17–19]

$$u_I(Z_i) = u(Z_i), \quad i = 1, 2, 3, 4,$$

$$\int_{\ell_i} (u_I - u) v = 0, \quad \forall v \in P_{k-2}(\ell_i), \quad i = 1, 2, 3, 4,$$

$$\int_e (u_I - u) v = 0, \quad \forall v \in Q_{k-2},$$

where $Z_i$ and $\ell_i$ are the corners and edges of the element $e$ in Fig. 1. In what follows we assume that $k \geq 2$. From (2.8) we have,

$$\int_e (u_I - u) = 0,$$

because the set $Q_{k-2}$ always contains a constant. Denote $V^h_0 \subset H^1_0(S)$ as

$$V^h_0 = \{v | v \text{ satisfies (2.6)–(2.8) and } v|_{\partial S} = 0\}.$$
The bi-kth-order Lagrange elements for (1.1) read: To seek $u_h \in V_h^0$ such that

$$b(u_h, v) = g(v), \quad \forall v \in V_h^0,$$

(2.10)

where

$$b(u, v) = \iint_S \nabla u \cdot \nabla v, \quad g(v) = \iint_S g v.$$

(2.11)

Since the interpolant $u_1$ in (2.6)-(2.8) is evaluated at the corners, on the edges, and in the area of the element $e = \square_{ij}$, we refer to it as the point-line-area interpolant, which is different from the point-wise Lagrange interpolant in the traditional bi-kth-Lagrange elements [20].

Now we assume that (1.2) has a positive solution curve $c$ with folds. Let $(\lambda^*, u^*)$ be the first fold on $c$, and $\lambda_0 \in [0, \lambda^*)$ be given. The weak form solution of (1.2) reads: To find $u_0 \in H_0^1(S)$ such that

$$\iint_S \nabla u_0 \cdot \nabla v - \lambda_0 \iint_S f(u_0) v = 0, \quad \forall v \in H_0^1(S).$$

(2.12)

Then the FEM solution reads: To seek $u_h \in V_h^0$ such that

$$\iint_S \nabla u_h \cdot \nabla v - \lambda_0 \iint_S f(u_h) v = 0, \quad \forall v \in V_h^0.$$

(2.13)

Suppose that the function $f(u)$ in (1.2) satisfies the following assumptions; see [21], pp. 508–509.

**A1.** $\|f\|_\infty \cdot \|Df\|_\infty \leq C$, where $\|Df\|_\infty = \max_{(x,y) \in S, 0 \leq u(x,y) < c_0} |Df(u)|$, and $c_0$ is a constant.

**A2.** $f(0) > 0$ in $S$.

**A3.** $Df(u) > 0$ for $u > 0$.

**A4.** $Df(u)$ is strictly increasing with respect to $u > 0$.

For superconvergence we need a stronger assumption than A1.

**A5.** Suppose $D^{\ell+1}f(u)$ is continuous and bounded, i.e.,

$$\|D^{\ell+1}f\|_\infty = \max_{(x,y) \in S, 0 \leq u(x,y) \leq c_0} |D^{\ell+1}f(u)| < C,$$

(2.14)

where $c_0$ and $C$ are constants.

Denote the Frechét derivative in (1.2) by $-\Delta - \lambda Df(u)$, where $Df(u) = f'(u)$ is the derivative of $f(u)$. It is well known that the operator $-\Delta - \lambda Df(u)$ is nonsingular at $(\lambda, u)$ if $\lambda < \lambda^*$, and is singular at the fold $(\lambda^*, u^*)$. Actually, $\lambda^*$ is the smallest eigenvalue of the eigenvalue problem

$$-\Delta \phi - \lambda^* Df(u^*) \phi = 0,$$

(2.15)

where $\phi$ is the eigenfunction corresponding to $\lambda^*$. Hence we have

$$\lambda^* = \min_{0 \neq \phi \in H_0^1(S)} \frac{\iint_S \nabla \phi \cdot \nabla \phi}{\iint_S Df(u^*) \phi^2}.$$

(2.16)

Suppose that (1.2) comes from a physical model which describes the temperature distribution of an object heated by an electric current, where only the positive temperature $u$ is of interest. It is well known that there exists a limit value $\lambda^*$ such that no temperature distribution goes beyond $\lambda^*$. Moreover, the function $f(u)$ may satisfy the following assumptions; see [21], pp. 508–509.

Assume that $f(u)$ satisfies A1–A5. We define the continuous linear operator $T : f \in L^2(\Omega) \rightarrow Tf = u_0 \in H_0^1(\Omega)$ which maps $f$ onto the solution $u_0$ of (2.12). Then $\lambda^*$ is bounded by $\mu_1$, the principal eigenvalue of the linear eigenvalue problem

$$\phi = \mu_1 T Df(0) \phi.$$

Compared with (2.15) the differentiation $Df(0)$ is independent of $u$. See [21], pp. 511–512. Hence for the solution $(\lambda, u)$ of (1.2), we have

$$0 \leq \lambda < \lambda^* \leq \mu_1.$$

(2.17)

Let $(\lambda, u(\lambda))$, $\lambda \in [0, \lambda^*)$ be a regular isolated solution. We may rewrite (2.12) and (2.13) as follows: To seek $u \in H_0^1(S)$ such that

$$a(u, v) = 0, \quad \forall v \in H_0^1(S),$$

(2.18)

and to seek $u_h \in V_h^0$ such that

$$a(u_h, v) = 0, \quad \forall v \in V_h^0.$$

(2.19)
Theorem 2.1. Let $A_1, A_5$ with $\ell = 1$, and $A_6$ hold for $v = u_I$ and $w = u_h$, where $u_I$ is the point-line-area interpolant of the true solution $u$ defined by (2.6)-(2.8), and $u_h$ the solution of (2.13) associated with the parameter $\lambda$, obtained using the bi-$k$-Lagrange elements. Suppose $u \in H^{k+1}(S)$ and the uniform rectangular elements $\square_{ij}$ are used. Then there exists the bound

$$\|u_h - u_I\|_{1.5} \leq C \left\{ \sup_{\xi \in V_h^\circ \cap \mathbb{R}} \left| \int_S \nabla (u - u_I) \cdot \nabla \xi \right| \right\}^{1/2} + \lambda h^{k+2} \|D^2 f\|_{\infty} |u|_{k+1.5},$$

(2.22)

where $h$ is the maximal boundary length of $\square_{ij}$, $C$ is a constant independent of $h$, and $\|D^2 f\|_{\infty}$ is defined in (2.14).

Proof. Let $v = u_h$ and $w = u_I \in V_h^\circ$. Denote $\xi = u_h - u_I \in V_h^\circ$. We obtain from A6 and (2.20),

$$d_0 \|u_h - u_I\|_{1.5}^2 \leq a(u_h, \xi) - a(u_I, \xi) = \int S \nabla (u - u_I) \cdot \nabla \xi - \lambda \int S (f(u) - f(u_I)) \xi. \tag{2.23}$$

From A1 we have

$$\int S (f(u) - f(u_I)) \xi = \int S Df(\theta u + (1 - \theta) u_I)(u - u_I) \xi = \int S (u - u_I) g,$$

where $\theta \in [0, 1]$ and $g = Df(\theta u + (1 - \theta) u_I) \times \xi$.

(2.24)

Since $S = \bigcup_{ij} \square_{ij}$, we have

$$\int S (u - u_I) g = \sum_{ij} \int_{\square_{ij}} (u - u_I) g. \tag{2.25}$$

Define the piecewise average constant $\overline{g} = \frac{\int_{\square_{ij}} g}{|\square_{ij}|}$ in $\square_{ij}$. Then from (2.6)-(2.8) we have

$$\int S (u - u_I) \overline{g} = \sum_{ij} \int_{\square_{ij}} (u - u_I) \overline{g} = 0. \tag{2.26}$$

Hence from (2.26), (2.27), and the Schwarz inequality, we have

$$\left| \int S (f(u) - f(u_I)) \xi \right| = \left| \sum_{ij} \int_{\square_{ij}} (u - u_I) (g - \overline{g}) \right| \leq \left\{ \sum_{ij} \int_{\square_{ij}} (g - \overline{g})^2 \right\}^{1/2} \times \left\{ \sum_{ij} \|u - u_I\|_{0, \square_{ij}}^2 \right\}^{1/2}. \tag{2.28}$$

From the approximation property of bi-$k$-Lagrange elements, we have

$$\|u - u_I\|_{1.5} = \left\{ \sum_{ij} \|u - u_I\|_{0, \square_{ij}}^2 \right\}^{1/2} \leq C h^{k+1} |u|_{k+1.5}. \tag{2.29}$$

Moreover, it follows from (2.25) that there exists the bound

$$|Dg| \leq \|D^2 f\|_{\infty} |\xi| + \|Df\|_{\infty} |D\xi|. \tag{2.30}$$

Then from the Schwarz inequality we have

$$\left\{ \sum_{ij} \int_{\square_{ij}} (g - \overline{g})^2 \right\}^{1/2} \leq C \left\{ \sum_{ij} \int_{\square_{ij}} |h| Dg | \right\}^{1/2} \leq C \left\{ \sum_{ij} \int_{\square_{ij}} (\|D^2 f\|_{\infty} |\xi| + \|Df\|_{\infty} |\xi|)^2 \right\}^{1/2} \leq C h^{1/2} \|D^2 f\|_{\infty} \|\xi\|_{1.5} \leq C h \|D^2 f\|_{\infty} \|\xi\|_{1.5} \leq C_1 h^{\frac{1}{2}} \|D^2 f\|_{\infty} \|\xi\|_{1.5}. \tag{2.31}$$
Proof. Let $\mathcal{C}_1$ be a constant independent of $h$. Combining (2.28), (2.29), and (2.31) leads to
\[
\left| \iint_S (f(u) - f(u_I)) \xi \right| \leq C h^{k+2} \| D^2 f \|_\infty \| u |_{k+1,5} \|_1,5.
\] (2.32)

Hence we have from (2.23) and (2.32),
\[
d_0 \| u_h - u_I \|^2_{1,5} \leq \iint_S \nabla (u - u_I) \cdot \nabla \xi + C h^{k+2} \lambda \| D^2 f \|_\infty \| u |_{k+1,5} \|_1,5.
\] (2.33)

The desired result (2.22) follows by dividing the two sides of the above equation by $\| \xi \|_{1,5}$ ($= \| u_h - u_I \|_{1,5}$). This completes the proof of Theorem 2.1. \(
\)

Assume that the bi-$k$-Lagrange elements are used with uniform rectangles. Based on the analysis of superconvergence for Poisson's equation [17,18], we have
\[
\sup_{\xi \in V_h} \left| \iint_S \nabla (u - u_I) \cdot \nabla \xi \right| \| \xi \|_{1,5} \leq C h^{k+2} \| u \|_{k+3,5}.
\] (2.34)

Hence if $u \in H^{k+3} (S)$, and $0 < \lambda \leq \lambda < \lambda^*$, where $\lambda^*$ is given in (2.17). From Theorem 2.1 we obtain the supercloseness,
\[
\| u_h - u_I \|_{1,5} = O (h^{k+2}).
\] (2.35)

For the bi-$k$-order Lagrange elements, we may formulate the a posteriori interpolant $I^k_p u_h$ of order $k + 2$ [2.4],
\[
\| u - I^k_p u_h \|_{1,5} = O (h^{k+2}).
\] (2.36)

Noting the optimal rate $O (h^2)$ in $H^1$ norm, the convergence rate in (2.36) may raise up to two orders $O (h^3)$. Such superconvergence rate is a significant improvement compared to that of [1], which is only one order (or a half order) higher than that of the $k$th-order Lagrange elements.

Since the integration $\iint_S f(u_I) v$ in (2.13) cannot be evaluated exactly, an approximation of the integration is necessary in practical computations. We modify (2.13) as: To seek $u_h \in V_h$ such that
\[
a_h(u_h, v) = \iint_S \nabla u_h \cdot \nabla v - \lambda \iint_S f(u_I) v = 0, \quad \forall v \in V_h^h,
\] (2.37)

where the rule of integration is chosen as
\[
\iint_S u v = \iint_S \hat{u} \hat{v},
\] (2.38)

with $\hat{u}$ and $\hat{v}$ the bi-$k$-order polynomial interpolants of $u$ and $v$, respectively. Note that for $v \in V_h^h$ we have $\hat{v} = v$. We give a strong monotonicity for $a_h(u, v)$.

A7. There exists a positive constant $d_0$ independent of $h$ such that the strong monotonicity holds:
\[
d_0 \| v - w \|^2_{1,5} \leq a_h(v, v - w) - a_h(w, v - w), \quad \forall v, w \in V_h^h.
\] (2.39)

Then we have the following theorem.

**Theorem 2.2.** Let A1, A5, and A7 hold for $v = u_I$ and $w = u_I$, and $u_h$ is the solution of (2.37) by the bi-$k$-Lagrange elements. Suppose that $u \in H^{k+1} (S)$ and the uniform rectangular elements $\square_{ij}$ are used. There exists the bound
\[
\| u_h - u_I \|_{1,5} \leq C \left\{ \sup_{\xi \in V_h^h} \left| \iint_S \nabla (u - u_I) \cdot \nabla \xi \right| \| \xi \|_{1,5} + \lambda h^{k+2} \| D^2 f \|_\infty \| u |_{k+1,5} + \| D^{k+1} f \|_\infty \right\},
\] (2.40)

where $h$ is the maximal boundary length of $\square_{ij}$, $C$ is a constant independent of $h$, and $\| D^2 f \|_\infty$ is defined in (2.14).

**Proof.** Let $\hat{f}(u)$ denote the bi-$k$-order interpolant of $f(u)$. For the true solution $u$ we have
\[
a_h(u, v) = \iint_S \nabla u \cdot \nabla v - \lambda \iint_S f(u_I) v = \left( \iint_S \nabla u \cdot \nabla v - \lambda \iint_S f(u) v \right) + \lambda \iint_S (f(u) - \hat{f}(u)) v
\] (2.41)
Let \( v = u_h \), \( w = u_l \) \( \in \mathcal{V}_0^h \), and \( \xi = u_h - u_l \). From A7, (2.41), and (2.37) we obtain
\[
d_0 \| u_h - u_l \|^2_{1,5} \leq a_h(u_h, \xi) - a_h(u_l, \xi) = -a_h(u_l, \xi) + a_h(u_l, \xi) - \lambda \int_S (f(u) - \tilde{f}(u)) \xi
\]
\[
= \int_S \nabla(u - u_l) \cdot \nabla \xi - \lambda \int_S (\tilde{f}(u) - \tilde{f}(u_l)) \xi - \lambda \int_S (f(u) - \tilde{f}(u_l)) \xi
\]
\[
= \int_S \nabla(u - u_l) \cdot \nabla \xi - \lambda \int_S (f(u) - \tilde{f}(u_l)) \xi
\]
\[
= \int_S \nabla(u - u_l) \cdot \nabla \xi - \lambda \left[ \int_S (f(u) - f(u_l)) \xi + \int_S (f(u_l) - \tilde{f}(u_l)) \xi \right].
\] (2.42)

The bounds of the first two terms on the most right-hand side of (2.42) have been derived in Theorem 2.1. Thus, we only need to derive the bound for the third term in (2.42). We have
\[
\int_S (f(u_l) - \tilde{f}(u_l)) \xi = \sum_{ij} \int_{\mathcal{D}_{ij}} (f(u_l) - \tilde{f}(u_l)) \xi.
\] (2.43)

Since \( f(u_l) \) and \( \tilde{f}(u_l) \) are highly continuous on \( \mathcal{D}_{ij} \), we have
\[
| f(u_l) - \tilde{f}(u_l) | \leq C h^{k+1} \| D^{k+1} f(u_l) \|_{\infty} \leq C_{1} h^{k+1} \| D^{k+1} f(u) \|_{\infty} = C_{1} h^{k+1} \| D^{k+1} f \|_{\infty},
\] (2.44)
by noting that \( u_l \) is close to \( u \), where \( C \) and \( C_1 \) are constants independent of \( h \). Moreover, we denote the piecewise average constant by \( \xi = \frac{1}{|\mathcal{D}_{ij}|} \) in \( \mathcal{D}_{ij} \). Based on (2.9), we have
\[
\int_{\mathcal{D}_{ij}} (f(u_l) - \tilde{f}(u_l)) \xi = 0.
\] (2.45)

Then we have from (2.43),
\[
\int_S (f(u_l) - \tilde{f}(u_l)) \xi = \sum_{ij} \int_{\mathcal{D}_{ij}} (f(u_l) - \tilde{f}(u_l)) \xi = \sum_{ij} \int_{\mathcal{D}_{ij}} (f(u_l) - \tilde{f}(u_l)) (\xi - \bar{\xi})
\]
\[
\leq C h^{k+1} \| D^{k+1} f \|_{\infty} \sum_{ij} \int_{\mathcal{D}_{ij}} |\xi - \bar{\xi}|.
\] (2.46)

Moreover, from the Schwarz inequality,
\[
\sum_{ij} \int_{\mathcal{D}_{ij}} |\xi - \bar{\xi}| \leq C \sqrt{|\mathcal{D}_{ij}|} \left( \sum_{ij} \|\xi - \bar{\xi}\|_{0, \mathcal{D}_{ij}}^2 \right)^{1/2} \leq C_1 h \left( \sum_{ij} \|\xi\|^2_{1, \mathcal{D}_{ij}} \right)^{1/2}
\]
\[
\leq C_1 h \|\xi\|_{1,5}.
\] (2.47)

where \( C_1 \) is also a constant independent of \( h \). Combining (2.44)-(2.47) gives
\[
\int_S (f(u_l) - \tilde{f}(u_l)) \xi \leq C h^{k+2} \| D^{k+1} f \|_{\infty} \|\xi\|_{1,5}.
\] (2.48)

From Theorem 2.1, (2.42), and (2.48) we obtain
\[
d_0 \| u_h - u_l \|^2_{1,5} \leq \int_S \nabla(u - u_l) \cdot \nabla \xi + C h^{k+2} \left( \| D^{k+1} f \|_{\infty} \|\xi\|_{1,5} + \| D^{k+1} f \|_{\infty} \right) \|\xi\|_{1,5}.
\]

The desired result (2.40) follows. This completes the proof of Theorem 2.2. □

Now we consider the strong monotonicity A6 and A7 for \( v = u_h \) and \( w = u_l \). Here we state two theorems without proofs, since the proofs are similar to those in [1], except that the regular triangles \( \mathcal{D}_{ij} \) are replaced by the uniform rectangles \( \mathcal{D}_{ij} \).

**Theorem 2.3.** Assume that A1–A4 and A5 hold for \( \ell = 1 \). Suppose that \( \lambda \in [0, \lambda^*], \hat{\lambda} < \lambda^*, u \in H^{k+1}(S) \), and that the quasi-uniform elements \( \mathcal{D}_{ij} \) are used. If \( h \) is small enough, the strong monotonicity A6 holds for \( v = u_h \) and \( w = u_l \), i.e.,
\[
a(u_h, u_h - u_l) - a(u_l, u_h - u_l) \geq d_0 \| u_h - u_l \|^2_{1,5},
\]
where \( d_0 \) is a positive constant independent of \( h \).
Theorem 2.4. Assume that A1–A4 and A5 hold. Suppose that \( \lambda \in [0, \lambda_0], \lambda < \lambda^*, u \in H^{k+1}(S) \), and that the quasi-uniform elements \( \Diamond \) are used. If \( h \) is small enough, the strong monotonicity A7 holds for \( v = u_h \) and \( w = u_i \), i.e.,
\[
a_h(u_h, u_h - u_i) - a_h(u_i, u_h - u_i) \geq d_0 \| u_h - u_i \|^2_{1,S}.
\]
where \( d_0 \) is a positive constant independent of \( h \).

3. A continuation algorithm using biquadratic Lagrange elements

In the superconvergence analysis for Poisson’s equation in [2–4,17,18], the main and key work is to derive the bound of
\[
\sup_{\xi \in V_h^0} \frac{\| \int_S \nabla(u - u_1) \cdot \nabla \xi \|}{\| \xi \|_{1,S}}.
\]
Since the strong monotonicity assumption for \( a(u, v) \) is confirmed from Theorems 2.3 and 2.4, the supercloseness \( \| u_1 - u_h \|_{1,S} = O(h^{k+2}) \)
is obtained directly from Theorems 2.1 and 2.2, and the superconvergence \( \| u - p_h \|^2_{2,h} \) follows. For the bi-kth-order Lagrange elements, the superconvergence \( O(h^{k+2}) \) in \( H^1 \) norm is two orders higher than the optimal convergence rate \( O(h^k) \) in [20]. Since rectangular domains are widely used in parameter-dependent problems, it is convenient to choose rectangular elements. We will use the biquadratic (i.e., bi-2) Lagrange elements to provide the detailed algorithms.

3.1. Biquadratic Lagrange elements

Consider Poisson’s equation with Dirichlet boundary conditions (see Fig. 2):
\[
-\Delta u = - \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = f(x, y) \quad \text{in } S,
\]
\[
u = g(x, y) \quad \text{on } \partial S,
\]
where \( S \) is a rectangle with boundary \( \partial S \), and \( f \) and \( g \) are smooth functions.

Denote the space \( H^1_0(S) = \{ v \mid v, \nu_x, \nu_y \in L^2(S), \nu|_{\partial S} = g \} \). We may rewrite (3.1) as a weak form: To seek \( u \in H^1_0(S) \) such that
\[
b(u, v) = \int_S f v, \quad \forall v \in H^1_0(S),
\]
and
\[
b(u, v) = \int_S \nabla u \cdot \nabla v,
\]
where \( \nabla u = u_i \mathbf{i} + u_j \mathbf{j} \), and \( \mathbf{i} \) and \( \mathbf{j} \) are the unit vectors along the \( x \)- and \( y \)-axis, respectively.

Now, we consider the biquadratic Lagrange elements on rectangles. Choose \( u_1 \in Q_2(x, y) = \text{span}\{1, x, y, xy, x^2, y^2, x^2 y, x y^2, x^2 y^2\} \) and \( v \in Q_2(x, y) \), where \( u_1 \) and \( v \) are the interpolant solution and the admissible function, respectively. The function \( v \) is formulated in the same way as \( u_i \). In this section, we formulate \( u_i \in Q_2 \) and \( v \in Q_2 \) by means of the point-line-area interpolant which was first introduced in [22]. The piecewise interpolant functions \( u_i \in Q_2(x, y) \) are defined as follows:
\[
u_i(Z_i) = u(Z_i), \quad i = 1, 2, 3, 4,
\]
\[
\int_{u_r \cap \Diamond} (u - u_i) d\ell = 0, \quad r = 1, 2, 3, 4,
\]
\[
\int_{\Diamond} (u - u_i) d\ell = 0.
\]

Obviously (3.4)–(3.6) are a special case of (2.6)–(2.8) with \( k = 2 \). Hence, the interpolant functions \( u_i \) on \( \Diamond \) are designed based on the solutions evaluated at the corners \( Z_i \) \( (i = 1, 2, 3, 4) \), on the integrals along the four edges \( \xi_i \) \( (i = 1, 2, 3, 4) \) of \( \partial \Diamond \), and on the area integral on \( \Diamond \). On the other hand, the traditional Lagrange interpolants with order two are defined on rectangles \( \Diamond \), by means of nodal values.
at the corners $Z_i$ ($i = 1, 2, 3, 4$), at the midpoints of the edges $\partial Q_{ij}$, and at the centroid of $Q_{ij}$. To link the two interpolation methods on $Q_{ij}$, the point-line-area variables may be viewed as the corner values, the mean values along edges on $\partial Q_{ij}$, and the mean value on $Q_{ij}$.

Let the domain $S$ be split into small rectangles $\square ij$, i.e., $S = \bigcup_{ij} \square ij$. Denote by $h_i$ and $k_j$ the boundary lengths of $\square ij$, and $h = \max_i h_i, k_j$. The rectangles $\square ij$ are said to be quasi-uniform if

$$\frac{h}{\min_{i,j} (h_i, k_j)} \leq \bar{c},$$

for some constant $\bar{c}$ independent of $h$. The quasi-uniform elements are said to be uniform if $h_i = h$ and $k_j = k$. Without loss of generality we assume $h \geq k$. Let us give explicitly the nine basis functions of the biquadratic Lagrange elements. Denote $\square ij = ((x, y) | x_i \leq x \leq x_{i+1}, y_j \leq y \leq y_{j+1})$, and choose the affine transformations: $\xi = \frac{x-x_i}{h_i}$ and $\eta = \frac{y-y_j}{k_j}$, where $h_i = x_{i+1} - x_i$ and $k_j = y_{j+1} - y_j$. Then the admissible functions on $\square ij$ can be expressed as

$$v(x, y) = \sum_{i=1}^{4} v_{ij}(\xi, \eta) + \sum_{t=1,3} \left( \int_{\ell_t} \frac{v}{h_t} \right) \psi_t(\xi, \eta) + \sum_{i=2,4} \left( \int_{\ell_t} v \right) \psi_t(\xi, \eta) + \left( \int_{Q_{ij}} v \right) \phi_t(\xi, \eta),$$

where the indices $1, 2, 3, 4$ denote $(i, j), (i+1, j), (i, j+1), (i+1, j+1)$, respectively; see Fig. 2. The integrals $\frac{1}{h_t} \int_{\ell_t} v, \frac{1}{k_j} \int_{\ell_k} v, \frac{1}{h_t} \int_{\ell_t} v$, and $\frac{1}{h_t} \int_{\ell_t} v$ are also regarded as the mean values of $v$ along the edges $\ell_t$, and $\frac{1}{h_t} \int_{\ell_t} v$ is regarded as the mean value of $v$ on $\square ij$. The nine basis functions on $[0, 1]^2$ are given explicitly by

$$\phi_1(x, y) = (1 - 3x)(1 - y)(1 - y),$$
$$\phi_2(x, y) = x(3x - 2)(1 - 3y)(1 - y),$$
$$\phi_3(x, y) = (1 - 3x)(1 - x)(3y - 2)y,$$
$$\phi_4(x, y) = x(2 - 3x)(2 - 3y)y,$$
$$\phi_5(x, y) = \psi_1(x, y) = 6x(x - 1)(2 - 3y)y,$$
$$\phi_6(x, y) = \psi_2(x, y) = 6x(3x - 2)(1 - y)y,$$
$$\phi_7(x, y) = \psi_3(x, y) = 6x(1 - x)(1 - y)(1 - y),$$
$$\phi_8(x, y) = \psi_4(x, y) = 6(1 - 3x)(1 - x)(1 - y)y,$$
$$\phi_9(x, y) = \psi_5(x, y) = 36x(1 - x)(1 - y)y.$$

Let $\bar{V}^h = \{v \in L^2(S) | v|_{\partial S} = g_I\}$. The biquadratic Lagrange elements for (3.1) and (3.2) are designed to seek $u_h \in \bar{V}^h$ such that

$$b(u_h, v) = \int_S f v, \quad \forall v \in \bar{V}^h.$$

We will employ the a posteriori interpolant to obtain global ultraconvergence results. The a posteriori interpolant may be formulated based on the computed solution $u_h$ as follows: $\Pi^h v \in Q_4(x, y)$ on $\square_{2i+1,2j+1}$, where $Q_4(x, y) = \sum_{t,j=0} a_{ij} x^t y^j$ with coefficients $a_{ij} \in \mathbb{R}$. Therefore, there are 25 coefficients in $\Pi^h v$, which can be determined uniquely by the following 25 equations (see Fig. 3):

$$v(G_t) = (\Pi^h v)(G_t), \quad t = 1, 2, \ldots, 9,$$
$$\int_{\ell_t} v = \int_{\ell_t} \Pi^h v, \quad r = 1, 2, \ldots, 12,$$
$$\int_{S_t} v = \int_{S_t} \Pi^h v, \quad t = 1, 2, 3, 4.$$

![Fig. 3. Diagram](image-url)

![Fig. 4. Diagram](image-url)
The computational formulas are expressed as
\[ I_p^v(x, y) = \sum_{i=1}^{9} v(G_i)\phi_i^*(\xi, \eta) + \sum_{i=1}^{6} \frac{f_{\ell_i}^v}{h}\psi_i^*(\xi, \eta) + \sum_{i=1}^{12} \frac{f_{k_i}^v}{k}\eta_i^*(\xi, \eta) + \sum_{i=1}^{4} \frac{f_{\ell_5}^v}{h}\phi_i^*(\xi, \eta), \] (3.12)
where \( \xi = \frac{x-x_1}{x_2-x_1} \) and \( \eta = \frac{y-y_1}{y_2-y_1} \). In (3.12), \( G_i \), \( \ell_i \), and \( S_i \) denote the vertices, edges, and areas of \( \square_{ij} \), respectively, as shown in Fig. 3.

The 25 basis functions \( \phi_i^*, \psi_i^*, \) and \( \varphi_i^* \) on \([0, 2]^2\) can be obtained explicitly from (3.9)-(3.11) using Mathematica. First, we obtain the point-line-area Lagrange interpolant with order four on \( \phi \).

\[ v(x) = \sum_{i=1}^{3} v(G_i)\varphi_i(x) + \left( \int_{\ell_1} v \right)\varphi_4(x) + \left( \int_{\ell_2} v \right)\varphi_5(x), \]

where the five basis functions on \([0, 2]\) are given explicitly by
\[
\begin{align*}
\varphi_1(x) &= \frac{1}{4} (x - 1)(x - 2)(5x^2 - 9x + 2), \\
\varphi_2(x) &= x(x - 2)(5x^2 - 10x + 4), \\
\varphi_3(x) &= \frac{1}{4} x(x - 1)(5x^2 - 11x + 4), \\
\varphi_4(x) &= -\frac{1}{4} x(x - 1)(x - 2)(15x - 23), \\
\varphi_5(x) &= -\frac{1}{4} x(x - 1)(x - 2)(15x - 7).
\end{align*}
\]

Then the 25 basis functions \( \phi_i^*, \psi_i^*, \) and \( \varphi_i^* \) in (3.12) on \([0, 2]^2\) can be obtained by the tensor products of \( \varphi_i \).

If uniform rectangular elements are used for the bi-quadratic elements (i.e., the bi-2 degree finite elements), we obtain the following superconvergence in [4],
\[
\frac{\int f_v (u - u_h) \cdot \nabla w}{\|w\|_{1,5}} \leq C h^4 \|u\|_{5,5}, \quad \forall w \in H_0^1(S),
\] (3.13)
where \( h \) is defined in (3.7). Eq. (3.13) indicates that the convergence rate of the bi-quadratic elements is two orders higher than the optimal convergence rate \( O(h^2) \). It is interesting to see that with uniform elements \( \square_{ij} \) for the special case \( f_{xxyy} = 0 \), there exists the ultra-convergence [4]
\[
\frac{\int f_v (u - u_h) \cdot \nabla w}{\|w\|_{1,5}} \leq C h^4 \|u\|_{6,5}, \quad \forall w \in H_0^1(S),
\] (3.14)
which are three orders higher than \( O(h^5) \) ! Using an a posteriori interpolant polynomial \( I_p^u u_h \) of order six on \( 3 \times 3 \) rectangles \( \square_{ij} \) in [4], the global ultra-convergence \( O(h^5) \) can be achieved.

The case \( f_{xxyy} = 0 \) in (3.1) implies that
\[
f(x, y) = f_1(x)p_1(y) + p_1^*(x)f_2(y),
\] (3.15)
where \( p_1(y) \) and \( p_1^*(x) \) are linear functions, and \( f_1(x) \) and \( f_2(y) \) are any smooth functions. For the parameter-dependent problem (1.2), however, there exists the case
\[
\frac{\partial^4}{\partial x^2 \partial y^2} f(u) \neq 0,
\] (3.16)
since its solution \( u \) is not in the form of (3.15), in general. Hence, the ultra-convergence in (3.14) is invalid for (1.2), and our target for superconvergence is to pursue the \( O(h^6) \) from (3.13) only.

Based on Theorems 2.1, 2.2, and (3.13), we have the following result.

**Theorem 3.1.** Assume that \( A1-A7 \) hold. Suppose that \( \lambda \in [0, \bar{\lambda}], \bar{\lambda} < \lambda^*, u \in H^6(S) \), and that the uniform elements \( \square_{ij} \) are used for the bi-quadratic Lagrange elements. If (2.37) is estimated using integration approximations, then for the parameter-dependent problem (1.2) there exists the following superconvergence
\[
\|u_l - u_h\|_{1,5} = O(h^4), \quad \|u - I_p^u u_h\|_{1,5} = O(h^6),
\]
where \( h \) is the maximal boundary of \( \square_{ij} \).

### 3.2. A continuation algorithm

In general the solution curve of (1.2) is traced numerically by a predictor–corrector continuation method. But first of all, we have to discretize the PDE, say, by the finite differences or the finite elements. Assume that a parametrization via arclength is available on the
Eq. (3.20) is the discrete formulation of (3.17) with the additional constraint condition. Here we use the tangent vector

\[ \mathbf{u}_h \]

the constraint vector. Then the predicted point in the

\[ \mathbf{u}_h \]

The second equation of (3.22) means that the Newton iteration is performed in the hyperplane which is perpendicular to the tangent vector \( \mathbf{u}_h \).

\[ \lambda(\mathbf{u}_h, w) = 0 \]

Suppose that in the \( k \)th step of the predictor-corrector continuation algorithm, a point \( (\mathbf{\lambda}_h^{(k)}, \mathbf{u}_h^{(k)}) \in \mathbb{R} \times \mathbb{V}_h^b \) which has been accepted as an approximating point for the solution curve \( c \). Then in the \( (k+1) \)th step of the continuation algorithm, we compute the tangent vector \((\mathbf{\lambda}_h^{(k+1)}, \mathbf{u}_h^{(k+1)})\) at \((\mathbf{\lambda}_h^{(k)}, \mathbf{u}_h^{(k)})\) by solving

\[
\left\{ \begin{array}{l}
\iint_{S} \nabla \mathbf{u}_h^{(k+1)} \cdot \nabla \mathbf{v} - \lambda_h^{(k+1)} \iint_{S} f' \mathbf{u}_h^{(k+1)} \mathbf{v} = 0 \quad \text{for all } \mathbf{v} \in \mathbb{V}_h^b, \\
\| (\mathbf{\lambda}_h^{(k+1)}, \mathbf{u}_h^{(k+1)}) \|_2 = 1.
\end{array} \right.
\]

Eq. (3.19) is equivalent to the following bordered matrix formulation

\[
\begin{bmatrix}
D_x F(\mathbf{\lambda}_h^{(k)}, \mathbf{u}_h^{(k)}) & D_u F(\mathbf{\lambda}_h^{(k)}, \mathbf{u}_h^{(k)}) \\
\hat{\mathbf{\lambda}}_h^{(k)} & \hat{\mathbf{u}}_h^{(k)}
\end{bmatrix}
\begin{bmatrix}
\hat{\mathbf{\lambda}}_h^{(k+1)} \\
\hat{\mathbf{u}}_h^{(k+1)}
\end{bmatrix}
= \begin{bmatrix} 0 \\ 1 \end{bmatrix},
\]

where \( D_x F(\mathbf{\lambda}_h^{(k)}, \mathbf{u}_h^{(k)}) \) corresponds to the discretization of the operator \(-\Delta - \lambda_h^{(k)} f' \mathbf{u}_h^{(k)}\), and \( D_u F(\mathbf{\lambda}_h^{(k)}, \mathbf{u}_h^{(k)}) = -f \mathbf{u}_h^{(k)}\). Actually, Eq. (3.20) is the discrete formulation of (3.17) with the additional constraint condition. Here we use the tangent vector \((\hat{\mathbf{\lambda}}_h^{(k)}, \hat{\mathbf{u}}_h^{(k)})\) as the constraint vector. Then the predicted point in the \( (k+1) \)th step continuation algorithm is obtained by setting

\[
(\mathbf{\lambda}_h^{(k+1)}, \mathbf{u}_h^{(k+1)}) = (\hat{\mathbf{\lambda}}_h^{(k)}, \hat{\mathbf{u}}_h^{(k)}) + \delta t (\hat{\mathbf{\lambda}}_h^{(k+1)}, \hat{\mathbf{u}}_h^{(k+1)}),
\]

where \( \delta t > 0 \) is the step length which is determined by some step-size selection strategy.

In the corrector step of the continuation algorithm, we perform Newton’s method to obtain the next approximating point \((\mathbf{\lambda}_h^{(k+1)}, \mathbf{u}_h^{(k+1)})\). More precisely,

\[
\int \int_{S} \nabla \mathbf{w}_j \cdot \nabla \mathbf{v} - \lambda_h^{(k+1), j} \iint_{S} f' \mathbf{u}_h^{(k+1), j} \mathbf{v} = - \iint_{S} f \mathbf{u}_h^{(k+1), j} \mathbf{v} \quad \text{for all } \mathbf{v} \in \mathbb{V}_h^b, \quad j = 1, 2, \ldots.
\]

The second equation of (3.22) means that the Newton iteration is performed in the hyperplane which is perpendicular to the tangent vector \((\hat{\mathbf{\lambda}}_h^{(k+1)}, \hat{\mathbf{u}}_h^{(k+1)})\). Then we set

\[
(\mathbf{\lambda}_h^{(k+1), j+1}, \mathbf{u}_h^{(k+1), j+1}) = (\mathbf{\lambda}_h^{(k+1), j}, \mathbf{u}_h^{(k+1), j}) + (\mu_j, \mathbf{w}_j), \quad j = 1, 2, \ldots.
\]
Fig. 6. The contour of $u$ at $\lambda = 3.4308863$ on the first solution branch of (5.1), where $V(x, y) = (x^2 + y^2)/2$ and $\mu = 30$.

Fig. 7. The contour of $u$ at $\lambda = -42.07593804$ on the first solution branch of (5.1), where $V(x, y) = (x^2 + y^2)/2$ and $\mu = -30$.

Table 1

<table>
<thead>
<tr>
<th></th>
<th>$d_1 = d_2 = 3$</th>
<th>$d_1 = d_2 = 3/2$</th>
<th>$d_1, d_2 = 3$</th>
<th>$d_1, d_2 = 3/2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>128.4301638434</td>
<td>274.6417543297</td>
<td>162.1534485313</td>
<td>365.0179733399</td>
</tr>
<tr>
<td>2</td>
<td>132.9297993120</td>
<td>275.7974378965</td>
<td>164.1534265302</td>
<td>366.1736569067</td>
</tr>
<tr>
<td>3</td>
<td>132.9297993120</td>
<td>275.7974378965</td>
<td>164.1534487694</td>
<td>367.5647977940</td>
</tr>
<tr>
<td>4</td>
<td>132.9297993120</td>
<td>275.8336076258</td>
<td>166.6530839999</td>
<td>368.7204813608</td>
</tr>
<tr>
<td>5</td>
<td>132.9297993120</td>
<td>275.8336076258</td>
<td>166.6530840000</td>
<td>368.7204813608</td>
</tr>
<tr>
<td>6</td>
<td>137.4294347807</td>
<td>276.9531214633</td>
<td>168.6530619988</td>
<td>368.7566510900</td>
</tr>
<tr>
<td>7</td>
<td>137.4294347807</td>
<td>276.9531214633</td>
<td>168.6530619988</td>
<td>369.5571584145</td>
</tr>
<tr>
<td>8</td>
<td>137.4294347807</td>
<td>276.9892911926</td>
<td>168.6530842380</td>
<td>369.5571736397</td>
</tr>
<tr>
<td>9</td>
<td>137.4294347807</td>
<td>277.0254609219</td>
<td>168.6530842380</td>
<td>369.9489352180</td>
</tr>
</tbody>
</table>

If

$$\| F_h (\lambda^{(k+1), j0+1}, u_h^{(k+1), j0+1} ) \| < \varepsilon$$

(3.23)

for some $j_0 \in \mathbb{N}$, where $\varepsilon > 0$ is the accuracy for the Newton corrector. Then we set

$$(\lambda_h^{(k+1)}, u_h^{(k+1)}) = (\lambda_h^{(k+1), j0+1}, u_h^{(k+1), j0+1}).$$

If (3.23) is not satisfied, we have to reduce the stepsize $\delta_k$ in (3.21), say, by half, and perform the Newton iteration again. We repeat the process described above until the solution curve we wish to follow is successfully traced.

In practical computations, Eq. (3.22) should be rewritten in the form similar to (3.20). We remark here that since $D_u F(\lambda, u)$ is symmetric, Eqs. (3.19) and (3.22) can be solved by using the block elimination algorithm. Finally, the linear systems may be solved using the preconditioned Lanczos method.

4. Efficient implementations of numerical continuation algorithms

As we may see from the numerical results in [15,16,23,24], in general, the energy levels of the NLS are far away from the corresponding bifurcation points on the trivial solution curve. This means that it might take more continuation steps to reach the target point, which in turn implies that the computational cost can be expensive even if we choose large enough step sizes. Thus, using numerical continuation methods to compute energy levels of NLS on a single grid is not recommended. To overcome the drawback we may apply the two-grid

If

$$\| F_h (\lambda_h^{(k+1), j0+1}, u_h^{(k+1), j0+1} ) \| < \varepsilon$$

(3.23)

for some $j_0 \in \mathbb{N}$, where $\varepsilon > 0$ is the accuracy for the Newton corrector. Then we set

$$(\lambda_h^{(k+1)}, u_h^{(k+1)}) = (\lambda_h^{(k+1), j0+1}, u_h^{(k+1), j0+1}).$$

If (3.23) is not satisfied, we have to reduce the stepsize $\delta_k$ in (3.21), say, by half, and perform the Newton iteration again. We repeat the process described above until the solution curve we wish to follow is successfully traced.

In practical computations, Eq. (3.22) should be rewritten in the form similar to (3.20). We remark here that since $D_u F(\lambda, u)$ is symmetric, Eqs. (3.19) and (3.22) can be solved by using the block elimination algorithm. Finally, the linear systems may be solved using the preconditioned Lanczos method.

4. Efficient implementations of numerical continuation algorithms

As we may see from the numerical results in [15,16,23,24], in general, the energy levels of the NLS are far away from the corresponding bifurcation points on the trivial solution curve. This means that it might take more continuation steps to reach the target point, which in turn implies that the computational cost can be expensive even if we choose large enough step sizes. Thus, using numerical continuation methods to compute energy levels of NLS on a single grid is not recommended. To overcome the drawback we may apply the two-grid
continuation schemes (TGCS) to trace solution curves of the NLS. The numerical results reported in [25] showed that a large amount of computational cost can be saved by implementing the two-grid schemes. Yet there is another possibility which can reduce the computational cost of the two-grid schemes. It was observed in [26] that we are only interested in the target point on the fine grid. Besides, the computations of two consecutive approximating points on the fine grid depend on their associated approximating points on the coarse grid and is independent to each other. This suggests that we may skip unnecessary computations of approximating points on the fine grid. Thus, we may trace a solution curve on the coarse grid until we are close enough to the target point. Then we apply the two-grid continuation scheme to compute the corresponding approximating points on the fine grid. We may proceed a few continuation steps to reach the target point on the fine grid if necessary. The procedure described above is referred to as “the simplified two-grid continuation scheme for computing energy levels of the BEC” [26].
Example 2. The choice of tolerances for the preconditioned Lanczos method and the Newton corrector are $0$ with uniform meshsize $\lambda$ ($\lambda, u$), where $V$.

Numerical results

The continuation algorithm described in Section 3 was implemented to computing energy levels and wave functions of the BEC. All test problems defined on the square domain were discretized by the biquadratic Lagrange elements with uniform meshsize. The accuracy tolerances for the preconditioned Lanczos method and the Newton corrector are $0.5 \times 10^{-9}$ and $0.5 \times 10^{-7}$, respectively. Our computations were executed on a Pentium 4 computer using FORTRAN 95 language with double precision arithmetic.

Example 1. We consider the following nonlinear Schrödinger eigenvalue problem

$$-\Delta u(x, y) - \mu u(x, y) + V(x, y)u(x, y) + \mu |u(x, y)|^2 u(x, y) = 0, \quad x \in \Omega = (-6, 6)^2,$$

$$u(x) = 0, \quad x \in \partial \Omega, \quad (5.1)$$

where $V(x, y) = (x^2 + y^2)/2$ and $\mu = 30, -30$. We chose the uniform meshsize $h = 12/32$. The first bifurcation point was detected at $(\lambda, u) \approx (1.41424963, 0)$. The solution curves of (5.1) on the $(\lambda, \|u\|)$-plane are shown in Fig. 5. The contours of the wave function at $\lambda = 3.43088630$ and $\lambda = -42.07593804$ are displayed in Figs. 6 and 7, where $\mu = 30$ and $\mu = -30$, respectively.

Example 2. We discretized the linear Schrödinger eigenvalue problem

$$-\Delta u(x, y) - \mu u(x, y) + \left[V(x) + a_1 \sin^2 \left(\frac{\pi x}{d_1}\right) + a_2 \sin^2 \left(\frac{\pi y}{d_2}\right)\right] u(x, y) = 0, \quad x \in \Omega = (-6, 6)^2,$$

$$u(x) = 0, \quad x \in \partial \Omega, \quad (5.2)$$

with uniform meshsize $h = 12/24$. Table 1 lists the first nine eigenvalues of (5.2) with $V(x, y) = (x^2 + y^2)/2, a_1 = a_2 = 3000$, and various choices of $d_1$ and $d_2$.

Example 3 (2D BEC in a periodic potential). We used the method described in Section 3 to compute the first two minimal energy levels of (1.9) with $V(x, y) = (x^2 + y^2)/2, a_1 = a_2 = 3000, \mu = 8$, and $\Omega = (-6, 6)^2$. The uniform meshsize for the biquadratic Lagrange elements is $h = 12/24$. The bifurcation points on the trivial solution curve $\{(\lambda, u) = (\lambda, 0) \mid \lambda \in \mathbb{R}\}$ are located at the eigenvalues of (5.2), see Table 1. Fig. 8 displays the first two solution curves with $d_1 = d_2 = 3$ and $d_1 = d_2 = 3/2$. Fig. 9 shows the contours of the ground-state solutions with $d_1 = d_2 = 3; d_1 = d_2 = 3/2; d_1 = 2, d_2 = 3; \text{and } d_1 = 1, d_2 = 3/2$. The contours of the first excited-state solutions with various choices of $d_1$ and $d_2$ are displayed in Fig. 10.
6. Conclusions

We have studied superconvergence of the bi-$k$-Lagrange elements for parameter-dependent problems, $k \geq 2$. The superconvergence rate of the bi-$k$-Lagrange elements is two orders higher than that of the $k$th-order Lagrange elements, which is a significant improvement of the previous results [1]. The bi-$k$-Lagrange elements have been applied to the computations of energy levels and wave functions of BEC, and BEC in a periodic potential, to provide satisfactory numerical solutions.

References