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Superconvergence of high order FEMs for eigenvalue problems with periodic boundary conditions

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ABSTRACT

We study Adini's elements for nonlinear Schrödinger equations (NLS) defined in a square box with periodic boundary conditions. First we transform the time-dependent NLS to a time-independent stationary state equation, which is a nonlinear eigenvalue problem (NEP). A predictor–corrector continuation method is exploited to trace solution curves of the NEP. We are concerned with energy levels and superfluid densities of the NLS. We analyze superconvergence of the Adini elements for the linear Schrödinger equation defined in the unit square. The optimal convergence rate $O(h^6)$ is obtained for quasiuniform elements. For uniform rectangular elements, the superconvergence $O(h^{6+p})$ is obtained for the minimal eigenvalue, where $p = 1$ or $p = 2$. The theoretical analysis is confirmed by the numerical experiments. Other kinds of high order finite element methods (FEMs) and the superconvergence property are also investigated for the linear Schrödinger equation. Finally, the Adini elements-continuation method is exploited to compute energy levels and superfluid densities of a 2D Bose–Einstein condensates (BEC) in a periodic potential. Numerical results on the ground state as well as the first few excited-state solutions are reported.

1. Introduction

During the past decade, Bose–Einstein condensates (BEC) in an optical lattice has been opening up intriguing possibilities for the study of coherent matter wave in periodic potentials [1–8]. The lattice potential is formed by overlapping two perpendicular optical standing waves with the BEC, which can be expressed as [7,8]

$$U(x,y) = U_0\{\cos^2(kx) + \cos^2(ky) + 2e_1 \cdot e_2 \cos\phi \cos(kx)\cos(ky)\}. \tag{1.1}$$

Here U_0 denotes the maximum potential of a single standing wave, $k = 2\pi/\mu$ is the magnitude of the wave vector of the lattice beams, with μ the wavelength generated by a near-infrared laser diode, e_1 and e_2 are the polarization vectors of the horizontal and vertical standing wave laser fields, respectively. The potential depth U_0 can be expressed in units of the recoil energy $E_r = \hbar^2k^2/2m$, where m is the mass of a single atom, e.g., rubidium. The variable ϕ denotes the time-phase difference between the two standing wave laser fields [9]. The governing equation for the BEC in a 2D optical lattice may be described by the nonlinear Schrödinger equation (NLS) or the Gross–Pitaevskii equation (GPE) [10,11]

$$\begin{aligned} &\mathbf{i}\Psi_t = -\frac{1}{2}\Delta\Psi + V(\mathbf{x})\Psi + U(\mathbf{x})\Psi + \mu|\Psi|^2\Psi, \quad \Psi > 0,\ \mathbf{x} \in \Omega \subset \mathbf{R}^2, \\ &\Psi(\mathbf{x},t) = 0, \quad \mathbf{x} \in \partial\Omega,\ t \geqslant 0. \end{aligned} \tag{1.2}$$

Here $\Psi = \Psi(\mathbf{x},t)$ is macroscopic wave function of the BEC with state variable $\mathbf{x} = (x,y)$, $V(\mathbf{x})$ the trapping potential, $U(\mathbf{x})$ the lattice potential defined in (1.1), μ a constant, and Ω a bounded domain in $\mathbf{R}^2$ with piecewise smooth boundary $\partial\Omega$. For convenience, we assume that Ω is a square box in this paper.

In [12], Wu and Niu studied superfluidity of a BEC in an optical lattice in one-dimension. Specifically, the Landau–Zener tunnelling and dynamical instability were investigated therein. Note that superflow of a BEC in an optical lattice is represented by a Bloch wave, a plane wave with periodic modulation of the amplitude.

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In this paper, we are concerned with energy levels and superfluid densities of a BEC in an optical lattice in two-dimension. The governing equation is

$$\mathbf{i}\Psi_t = -\frac{1}{2}\Delta\Psi + \widetilde{U}(x,y)\Psi + \mu|\Psi|^2\bar{\Psi} = 0 \quad \text{in } \Omega = (-\pi,\pi)^2, \qquad (1.3)$$
$$\Psi(x,y) = \Psi(x+2\pi,y) = \Psi(x,y+2\pi),$$

where $\widetilde{U}(x,y) = v_1 cos(\frac{x}{d_1}) + v_2 cos(\frac{y}{d_2})$ with d_i the distance between neighbor wells, v_i are positive constance, $i = 1,2$. We remark here that the trapping potential $V(\mathbf{x})$ in (1.2) is omitted in (1.3). Moreover, the Dirichlet boundary conditions in (1.2) is replaced by the periodic boundary conditions in (1.3).

An important invariant of the NLS is the mass conservation constraint, or the normalization of the wave function

$$\int_\Omega |\psi(\mathbf{x},t)|^2 d\mathbf{x} = 1, \quad t \geqslant 0. \qquad (1.4)$$

Various numerical methods have been proposed to study quantum behavior of the BEC, see e.g. [13–16]. By substituting

$$\Psi(\mathbf{x},t) = e^{-\mathbf{i}\lambda t}u(\mathbf{x}) \qquad (1.5)$$

into (1.3), we obtain the nonlinear eigenvalue problem

$$F(u,\lambda) = -\frac{1}{2}\Delta u(\mathbf{x}) - \lambda u(\mathbf{x}) + \widetilde{U}(\mathbf{x})u(\mathbf{x}) + \mu|u(\mathbf{x})|^2 u(\mathbf{x}) = 0 \quad \text{in } \Omega,$$
$$u(x,y) = u(x+2\pi,y) = u(x,y+2\pi). \qquad (1.6)$$

In general the function $u(\mathbf{x})$ in (1.5) is a complex function. For simplicity we assume $u(\mathbf{x})$ is a real function. Note that (1.6) is a parameter-dependent problem which can be solved using numerical continuation methods. For instance, Chien et al. proposed some variants of two-grid continuation schemes [17,18] to investigate energy levels and superfluid densities of rotating BEC [19].

The Schrödinger eigenvalue problem (SEP) associated with (1.6) is

$$-\frac{1}{2}\Delta u(\mathbf{x}) - \lambda u(\mathbf{x}) + \widetilde{U}(\mathbf{x})u(\mathbf{x}) = 0 \quad \text{in } \Omega = (-\pi,\pi)^2, \qquad (1.7)$$
$$u(x,y) = u(x+2\pi,y) = u(x,y+2\pi).$$

To compute an energy level of the GPE using numerical continuation methods, we may trace the corresponding solution curve branching from a bifurcation point on the trivial solution curve $\{(u,\lambda) = (0,\lambda)|\lambda \in \mathbf{R}\}$ of (1.6). We stop the curve-tracking whenever the constraint,

$$\int_\Omega |u(\mathbf{x})|^2 d\mathbf{x} = 1 \qquad (1.8)$$

is satisfied. The constraint (1.8) is referred to as a target point on the solution curve. Note that a bifurcation point of the GPE is just an eigenvalue of the associated SEP [20], which can be computed using numerical methods. Our aim is to study high order finite element methods (FEM) for the GPE. In particular, the Adini element approximations will be incorporated in the context of continuation methods for curve-tracking. Of particular interest here is the investigation of superconvergence for the simplified SEP

$$-\frac{1}{2}\Delta u = \lambda u \quad \text{in } \Omega = (-\pi,\pi)^2, \qquad (1.9)$$
$$u(x,y) = u(x+2\pi,y) = u(x,y+2\pi).$$

For eigenvalue problems of self-adjoint elliptic of differential operators, the finite element method was studied in Strang and Fix [21] and in Babuška and Osborn [22], and the error estimates were derived. The eigenvalue problems for algebraic equations and linear operators were also reported in Wilkinson [23] and Chatelin [24], respectively. Global superconvergence was developed for elliptic problems in Chen and Huang [25], Lin and Yan [26] and Yan [27], and applied for eigenvalue problems in Lin and Lin [28] and Yang [29]. We will discuss periodic eigenvalue problems given in [30], and employ the direct constraints in Li [31] to deal with periodic boundary conditions. Moreover, high order FEMs, such as Adini's elements, bi-quadratic and kth-order triangular elements, are chosen. We analyze superconvergence and derive new error bounds for high order FEMs.

In this paper we also give some numerical results of the Adini elements for the simplified SEP with different boundary conditions, i.e., Dirichlet, Neumann, periodic, and the Robin boundary conditions. Adini's elements are defined on rectangles $\square_{ij}$ with nodal variables, u, u_x and u_y, at four corners of $\square_{ij}$, and the interpolant functions are expressed by polynomials of $\widehat{P}_3 = P_3 + span\{x^3y, xy^3\}$, where $P_3 = \sum_{i+j=0}^{3} a_{ij}x^iy^j$ are cubic polynomials. Adini's elements were first studied in Adini and Clough [32] and Melosh [33]. In some literature, Adini–Clough–Melosh rectangle is called, see [34]. For simplicity, we call it Adini's elements in this paper. Error analysis of Adini's elements was given in many papers for the fourth order elliptic problems, e.g., the biharmonic equations. We only mention some of them: Lascaux and Lesaint [35], Kikuchi [36], and Miyoshi [37] and Ciarlet [34].

From the numerical results we obtain the superclose $\|u_I - u_h\|_0 = O(h^5)$ and $\|u_I - u_h\|_1 = O(h^4)$ for the uniform rectangles $\square_{ij}$, where u_I is Adini's interpolant based on the true solution u, and u_h the approximation solution for Adini's elements. By the a posteriori interpolant we get the global superconvergence $O(h^5)$ and $O(h^4)$ in L_2 norm and H_1 norm, respectively. Furthermore, we also obtain the convergence rate $O(h^6)$ of the minimal eigenvalue and the superconvergence $O(h^8)$ by the Rayleigh quotient based on the a posteriori interpolant in Yang [29]. Moreover, we can obtain higher accuracy and convergence rates by the extrapolation formulas based on the approximate eigenvalues.

This paper is organized as follows. In the next section, the linear eigenvalue problem (LEP) with Dirichlet and Neumann boundary conditions involving periodic boundary conditions is described, which are denoted by Models I and II, respectively. In Section 3, the Adini elements are employed for the LEP with Models I and II. In Section 4, superconvergence of Adini's elements by direct constraints is derived for Poisson's equation with Models I and II. In Section 5, the superconvergence is developed for LEP. In Section 6, the superconvergence is applied to other FEMs for Models I and II. In Section 7, numerical results are reported to support our theoretical analysis. Moreover, the ground state solutions as well as the first few excited-state solution of (1.6) are presented. Finally, some concluding remarks are given in Section 8.

2. Periodic boundary conditions

For convenience we rewrite (1.9) as

$$-\Delta u = \lambda u \quad \text{in } S = (0,1)^2, \qquad (2.1)$$
$$u^+ = u^-, \quad u_n^+ = u_n^- \quad \text{on } \Gamma^+, \qquad (2.2)$$

where $\Gamma = \partial S = \Gamma^+ \cup \Gamma^-$, $\Gamma^+ = \overline{BD} \cup \overline{CD}$, $\Gamma^- = \overline{AB} \cup \overline{AC}$, and $u^\pm = u|_{\Gamma^\pm}$ (see Fig. 1). In (2.2), we impose the normal derivative u_n ($u_x = \frac{\partial u}{\partial x}$ or $u_y = \frac{\partial u}{\partial y}$) on ∂S as shown in Fig. 1. because of finite element approximations. The simplified notations in (2.2) denote

$$u^+(x,1) = u^-(x,0), \quad u^+(1,y) = u^-(0,y) \qquad (2.3)$$

and

$$u_y^+(x,1) = u_y^-(x,0), \quad u_x^+(1,y) = u_x^-(0,y). \qquad (2.4)$$

Obviously, $\lambda = 0$ is the minimal eigenvalue of (2.1) and (2.2) with corresponding eigenfunction, $u \equiv constant$. We are interested in