Pseudospectral Methods for Computing the Multiple Solutions of the Schrödinger Equation

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Abstract. In this paper, we first compute the multiple non-trivial solutions of the Schrödinger equation on a square, by using the Liapunov-Schmidt reduction and symmetry-breaking bifurcation theory, combined with Legendre pseudospectral methods. Then, starting from the non-trivial solution branches of the corresponding nonlinear problem, we further obtain the whole positive solution branch with \(D_4\) symmetry of the Schrödinger equation numerically by pseudo-arclength continuation algorithm. Next, we propose the extended systems, which can detect the fold and symmetry-breaking bifurcation points on the branch of the positive solutions with \(D_4\) symmetry. We also compute the multiple positive solutions with various symmetries of the Schrödinger equation by the branch switching method based on the Liapunov-Schmidt reduction. Finally, the bifurcation diagrams are constructed, showing the symmetry/peak breaking phenomena of the Schrödinger equation. Numerical results demonstrate the effectiveness of these approaches.

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Key words: Schrödinger equation, multiple solutions, symmetry-breaking bifurcation theory, Liapunov-Schmidt reduction, pseudospectral method.

1 Introduction

As a canonical model in physics, the nonlinear Schrödinger equation (NLS) is of the form

\[
\begin{align*}
    i \frac{\partial}{\partial t} w(x,t) & = -\Delta w(x,t) + v(x)w(x,t) + \kappa g(x,|w(x,t)|)w(x,t), \\
    \frac{\partial}{\partial t} \int_{\mathbb{R}^n} |w(x,t)|^2 dx & = 0,
\end{align*}
\]

(1.1)

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where \( v(x) \) is a potential function, \( \kappa \) is a physical constant and \( g(x, u) \) is a nonlinear function satisfying certain growth and regularity conditions, e.g., \( g(x, |w|)w \) is super-linear in \( w \). The second equation in (1.1) is a conservation condition under which the NLS is derived, its solutions will be physically meaningful and the localized property will be satisfied. See [1]. Eq. (1.1) is called focusing for \( \kappa < 0 \) and defocusing for \( \kappa > 0 \), such as the well-known Gross-Pitaevskii equation in the Bose-Einstein condensate [1–5]. To study solution patterns, stability and other properties, solitary wave solutions of the form \( w(x, t) = u(x) e^{i\omega t} \) are investigated where \( \omega \) is a wave frequency and \( u(x) \) is a wave amplitude function. In such a case, the conservation condition in (1.1) will be automatically satisfied. Accordingly, \( u(x) \) satisfies the following semi-linear elliptic partial differential equation (PDE):

\[
\lambda u(x) = -\Delta u(x) + v(x)u(x) + \kappa g(x, |u(x)|)u(x).
\]

(1.2)

There are two types of multiple solution problems associated with (1.2): (i). one views \( \lambda \) as a given parameter and solves (1.2) for the multiple solutions \( u \); (ii). one views \( \lambda \) as an eigenvalue and \( u \) as the corresponding eigen-function, and solves (1.2) for the multiple eigen-solutions \( (\lambda, u) \).

For simplicity, let \( v(x) = 0 \) and \( \lambda \) be a parameter. The aim of this paper is to find the multiple solutions in \( H^0_\Omega \) of the following non-autonomous semilinear elliptic PDE:

\[
\begin{align*}
G(u(x),\lambda,r) & := -\Delta u(x) + \lambda u(x) + \kappa |x-x_0|^r |u(x)|^{p-1} u(x) = 0, & x \in \Omega, \\
u|_{\partial \Omega} & = 0,
\end{align*}
\]

(1.3)

where \( \Omega = [0,1] \times [0,1] \) is a square, \( x_0 = (0.5, 0.5) \), \( p > 1 \), \( \lambda, \kappa, r \) are prescribed parameters. Its variational functional is

\[
J(u) = \int_\Omega \left[ \frac{1}{2} (|\nabla u(x)|^2 + \lambda u^2(x)) + \frac{\kappa}{p+1} |x-x_0|^r |u(x)|^{p+1} \right] dx.
\]

(1.4)

The solutions of (1.3) correspond to the critical points \( u^* \) of \( J \), i.e., \( J'(u^*) = 0 \) in \( H = H^0_\Omega \). Denote by \( H = H^- \oplus H^0 \oplus H^+ \) the spectrum decomposition of \( J''(u^*) \), where \( H^- \), \( H^0 \), \( H^+ \) are respectively the maximum negative, null and maximum positive subspaces of the linear operator \( J''(u^*) \) with \( \text{dim} (H^0) < +\infty \). The quantity \( \text{dim}(H^-) \) is called the Morse Index (MI) of \( u^* \), and is denoted by \( \text{MI}(u^*) \). A critical point \( u^* \) with \( \text{MI}(u^*) = k \geq 1 \) is called an order \( k \)-saddle. Let \( 0 < \mu_1 < \mu_2 < \cdots \) be the eigenvalues of \( -\Delta \) satisfying the homogeneous Dirichlet boundary condition and \( \{v_1, v_2, \cdots \} \) be their corresponding eigenfunctions. The system (1.3) is called focusing (M-type) if \( \kappa < 0 \) and \( -\mu_{k+1} < \lambda < -\mu_k \), and defocusing (W-type) if \( \kappa > 0 \) and \( \mu_k < -\lambda < -\mu_{k+1} \). See [6]. The two cases are very different in both physical nature and mathematical structure. For both types, 0 is the only \( k \)-saddle. All non-trivial saddles have index \( k > k \) (\( k \) \) for M-type (W-type). In particular, for the M-type with \( \lambda > -\lambda_1 \), \( J \) is said to have a mountain pass structure and 0 is the only local minimum; for the W-type with \( k \geq 1 \), \( J \) has two local minima. In the literature, the two cases have to be treated by two very different types of variational methods.
The critical point theory has been applied to prove the existence and multiplicity of solutions of Eq. (1.3) under various assumptions. See [7, 8]. Particularly, the mountain pass theorem is very important for showing the existence of solutions of nonlinear equations. See [9]. In actual applications, due to the multiplicity, degeneracy and instability of the critical points with high Morse index, the computation of multiple solutions encounters essential difficulties. During the past few decades, a remarkable amount of progress has been made in the approximation approaches for the multiple solutions of some relevant problems. In the existing works, one usually computes multiple solutions using the scaling iterative algorithm, the monotone iteration, the direct iteration algorithm, or the research and extension method, cf. [10–14]. Unfortunately, the previous algorithms usually need a good guess of solution, which seems to be a difficult task.

To overcome this disadvantage, we shall use the bifurcation method [15–17] to compute the multiple solutions of (1.3). According to the bifurcation theory [18, 19], the equation (1.3) possesses nontrivial solutions, which can branch off from the bifurcation points. Thereby, we can find the multiple solutions of (1.3) by using the bifurcation method. In actual computations, the pseudospectral methods will be employed to compute the multiple solutions.

Theoretically, we can compute the multiple solutions of the equation (1.3) for any Morse index by using the finite difference method. However, with the improvement of the Morse index, the solution will oscillate rapidly. Particularly, the peak of the solution will occur at the boundaries as the Morse index of solutions growing very big. In this case, it is very hard to accurately simulate the behaviors of the solutions. Usually, one needs to refine the mesh, but the computational complexity is quite staggering. To overcome this deficiency, in this paper, we shall develop Legendre pseudospectral methods for computing the multiple solutions [20]. As we know that, the Legendre pseudospectral method is more accurate to the finite difference method [21], although its accuracy is degraded by corner singularities [22, 23].

The multiple solutions of the NLS have been considered by some researchers. For instance, Chien et al. [24–28] studied the bifurcation scenario of the NLS and the multilevel spectral-Galerkin continuation methods for parameter-dependent problems. Kevrekidis [29] presented the numerical continuation method for the discrete NLS. A general approach via continuation and multiple solution algorithms were given in [30]. The existence and symmetry properties of multi-bump solutions of the NLS were described in [31, 32]. The main numerical difficulties for the NLS (1.3) include: the equation is nonlinear and the solution will oscillate rapidly with big Morse index.

The aim of this paper is to propose an efficient Legendre pseudospectral method for the equation (1.3). The main differences between our new strategy and the existing ones are as follows:

(i) We compute the multiple solutions of the Schrödinger equation with a bigger Morse index and various symmetries, the existing works for the multiple solutions mainly deal with some partial differential equations with a smaller Morse index.
(ii) The suggested algorithms possess the high-order accuracy. Moreover, numerical experiments indicate that our method is much easier to find the nontrivial solutions, especially for the positive solutions.

(iii) We systematically discuss the symmetry breaking bifurcations about various parameters of the Schrödinger equation, and obtain the complete bifurcation diagram. In particular, we find out as many multiple solutions as possible.

(iv) The suggested algorithms can overcome effectively the difficulty for searching the initial guess encountered in some other popular algorithms.

The paper is organized as follows. In Section 2, we consider the multiple solutions of the Schrödinger equation (1.3) on a square. We describe an algorithm and establish Legendre pseudospectral scheme. In Section 3, the algorithms based on the bifurcation theory are applied to compute the positive solutions with \( D_4 \) symmetry of the problem (1.3). We take \( \lambda \) or \( r \) in the Schrödinger equation as a bifurcation parameter and propose the extended systems, which can detect the \( D_4 - \Sigma_d \) \((D_4 - \Sigma_1, D_4 - \Sigma_2, D_4 - \Sigma_M)\) symmetry-breaking bifurcation points on the branch of the \( D_4 \) symmetric positive solutions. The positive solutions with \( \Sigma_d \) \((\Sigma_1, \Sigma_2, \Sigma_M)\) symmetry are computed by the branch switching method based on the Liapunov-Schmidt reduction. Some numerical results are presented for the multiple positive solutions of the Schrödinger equation (1.3). The bifurcation diagrams are constructed, showing the symmetry/peak breaking phenomena of the Schrödinger equation. The final section is for some concluding discussions.

2 The multiple solutions of the Schrödinger equation (1.3) on a square

2.1 The equivariance properties and the symmetry-breaking bifurcation of (1.3)

We first discuss the symmetry properties of the problem (1.3).

The symmetry groups of a square are \( D_4 = \{I, R_1, R_2, R_3, S_1, S'_1, S_2, S'_2\} \) and \( \Gamma = D_4 \times Z_2 \), where

\[
\begin{align*}
Iu(x_1, x_2) &= u(x_1, x_2), & S_1u(x_1, x_2) &= u(x_1, 1- x_2), \\
S'_1u(x_1, x_2) &= u(1-x_1, x_2), & S_2u(x_1, x_2) &= u(1-x_2, x_1), \\
S'_2u(x_1, x_2) &= u(1-x_2, 1- x_1), & R_1u(x_1, x_2) &= u(1-x_2, x_1), \\
R_2u(x_1, x_2) &= u(1-x_1, 1- x_2), & R_3u(x_1, x_2) &= u(x_2, 1- x_1), \\
Z_2 &= \{I, -I\}.
\end{align*}
\]

If \( p \) in (1.3) is odd, namely,

\[
G(\gamma u, \lambda, r) = \gamma G(u, \lambda, r), \quad \forall \gamma \in \Gamma,
\]
then (1.3) is $\Gamma$-equivariant. Moreover, (1.3) is $D_4$-equivariant, provided that $p$ is even.

Particularly, the trivial solution $u$ in the reduced problem (2.1).

leads to the following reduced problems:

The solutions of (2.1) are precisely the solutions of (1.3) with at least the symmetry of $X^\Sigma$. The symmetry-breaking bifurcation theory [18, 19] indicates that if there exists a bifurcation point $\lambda = \lambda_0$ with the corresponding eigenfunction $\psi_0 \in X^\Sigma$, then the nontrivial solution branch of $\Sigma$ symmetry will bifurcate from the trivial solution at $\lambda = \lambda_0$. The reduced problem (2.1) will be very useful, since we only need to resolve the problem in one of the symmetry domains. However, in this case, the boundary conditions should be changed according to the underlying symmetry $\Sigma$. In Table 3 below, we describe the domains that need to resolve and the corresponding boundary conditions for various $\Sigma$ in the reduced problem (2.1).

<table>
<thead>
<tr>
<th>Fixed point spaces $X^{D_4}$</th>
<th>Orthogonal bases</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X^{d_4}$</td>
<td>$\sin(2k-1)\pi x_1 \sin(2k-1)\pi x_2$ or $\sin(2k-1)\pi x_1 \sin(2k-1)\pi x_2 + \sin(2k+1)\pi x_2 \sin(2k+1)\pi x_1$</td>
</tr>
</tbody>
</table>

Table 1: The fixed point spaces and their bases.
Table 2: The numbers and the symmetries.

<table>
<thead>
<tr>
<th>Bifurcation points</th>
<th>Nontrivial solution branches</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Numbers</td>
</tr>
<tr>
<td>$(2\pi^2,0)$</td>
<td>1</td>
</tr>
<tr>
<td>$(5\pi^2,0)$</td>
<td>2</td>
</tr>
<tr>
<td>$(8\pi^2,0)$</td>
<td>1</td>
</tr>
<tr>
<td>$(10\pi^2,0)$</td>
<td>2</td>
</tr>
<tr>
<td>$(13\pi^2,0)$</td>
<td>2</td>
</tr>
<tr>
<td>$(17\pi^2,0)$</td>
<td>2</td>
</tr>
<tr>
<td>$(18\pi^2,0)$</td>
<td>1</td>
</tr>
<tr>
<td>$(20\pi^2,0)$</td>
<td>2</td>
</tr>
<tr>
<td>$(25\pi^2,0)$</td>
<td>2</td>
</tr>
<tr>
<td>$(32\pi^2,0)$</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 3: The domains and the boundary conditions for various $\Sigma$.

<table>
<thead>
<tr>
<th>The symmetries</th>
<th>The domains</th>
<th>The boundary conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_1'$</td>
<td>$[0,\frac{1}{2}] \times [0,1]$</td>
<td>$u\big</td>
</tr>
<tr>
<td>$\Sigma_1$</td>
<td>$[0,1] \times [0,\frac{1}{2}]$</td>
<td>$u\big</td>
</tr>
<tr>
<td>$\Sigma_r$</td>
<td>$[0,\frac{1}{2}] \times [0,1]$</td>
<td>$u\big</td>
</tr>
<tr>
<td>$\Sigma_M$</td>
<td>$[0,1] \times [0,\frac{1}{2}]$</td>
<td>$u\big</td>
</tr>
<tr>
<td>$\Sigma_R$</td>
<td>$[0,\frac{1}{2}] \times [0,\frac{1}{2}]$</td>
<td>$u\big</td>
</tr>
<tr>
<td>$\Sigma_2$</td>
<td>$0 \leq x \leq 1$, $0 \leq y \leq x$</td>
<td>$u\big</td>
</tr>
<tr>
<td>$\Sigma'_2$</td>
<td>$0 \leq x \leq 1$, $1-x \leq y \leq 1$</td>
<td>$u\big</td>
</tr>
<tr>
<td>$\Sigma_d$</td>
<td>$0 \leq x \leq 1$, $0 \leq y \leq \frac{1}{2}$, $y \leq x$, $y \leq 1-x$</td>
<td>$u\big</td>
</tr>
<tr>
<td>$D_4$</td>
<td>$0 \leq x \leq \frac{1}{2}$, $0 \leq y \leq x$</td>
<td>$u\big</td>
</tr>
</tbody>
</table>

2.2 Algorithm descriptions

In this subsection, we resolve the nontrivial multiple solutions of the Schrödinger equation (1.3) on a square by using the Liapunov-Schmidt reduction and the numerical con-
continuation methods. Our process includes the following three steps:

(i) Use the Liapunov-Schmidt reduction principle (cf. [33–35]) to obtain the nontrivial solution branches near the bifurcation points. More precisely, let

\[ u = \tau \ast \psi_0 + w, \quad \eta = \lambda - \lambda_0, \]

where \( \lambda_0 \) is the eigenvalue of the operator \( \Delta \) on \( \Omega \), \( \psi_0 \) is the corresponding eigenfunction, \( w \) is an unknown function satisfying the orthogonal relationship

\[ \langle \psi_0, w \rangle = \int_{\Omega} \psi_0(x_1, x_2) w(x_1, x_2) dx_1 dx_2 = 0, \]

and \( \tau > 0 \) is a small parameter. Clearly, for \( \Omega = [0,1] \times [0,1] \), we have \( \lambda_0 := \lambda_{n,m} = (n^2 + m^2) \pi^2 \) and \( \psi_0 := \psi_{n,m} = \sin(n \pi x_1) \sin(m \pi x_2), n, m = 1, 2, 3, 4, \ldots \).

For a given small parameter \( \tau \), we first resolve numerically the following system of \( w \) and \( \eta \), by using Legendre pseudospectral method suggested in Subsection 2.3 and a Newton-Raphson iteration process with the initial data \( \eta = 0 \) and \( w = 0 \):

\[
\begin{cases}
-\Delta w + (\eta + \lambda_0)w + \eta \tau \psi_0 + \kappa|x - x_0|^{\nu} \tau \psi_0 + w|^{p-1}(\tau \psi_0 + w) = 0, & x \in \Omega, \\
w|_{\partial \Omega} = 0, \\
\int_{\Omega} \psi_0(x_1, x_2) w(x_1, x_2) dx_1 dx_2 = 0.
\end{cases}
\]

(ii) Denote by \( \eta_1 \) and \( w_1 \) the approximation solutions of \( \eta \) and \( w \) in (2.2). Then, increasing \( \tau \) gradually and resolving numerically the unknowns \( \eta \) and \( w \) in (2.2) and using the same process with the iterative initial data \( \eta_1 \) and \( w_1 \), we obtain new approximation solutions of \( \eta \) and \( w \). Repeat this process until the approximation solution of \( u \) is far away from the trivial solution.

(ii) Denote by \( \tau_{end}, \eta_{end} \) and \( w_{end} \) the final approximation solutions of \( \tau \), \( \eta \) and \( w \) in the previous process. Let

\[ u_{end} = \tau_{end} \ast \psi_0 + w_{end}, \quad \lambda_{end} = \lambda_0 + \eta_{end}. \]

For a given initial data \( \lambda = \lambda_{end} \), we then solve Eq. (1.3) of \( u \) numerically, using the suggested Legendre pseudospectral algorithm in Subsection 2.3 and a Newton-Raphson iteration process with the initial data \( u = u_{end} \).

(iii) Let \( u_1 \) be the approximation solution of \( u \) in the previous process. Then, decreasing \( \lambda \) gradually and resolving numerically the unknown \( u \) in (1.3) by using the same process with the iterative initial data \( u_1 \), we obtain a new approximation solution of \( u \). Repeat this process until \( \lambda \) is equal to the value \( \lambda \) given in (1.3).
2.3 Legendre pseudospectral scheme

In this subsection, we shall construct Legendre pseudospectral scheme (cf. [36–38]) for solving Eqs. (2.2) and (1.3).

Let \( \{ L_n(x) \}_{n \geq 0}, 0 \leq x \leq 1 \) be the standard Legendre polynomials. They satisfy the orthogonality relationship:

\[
\int_0^1 L_m(x)L_n(x)dx = \frac{1}{2n+1} \delta_{mn},
\]

where \( \delta_{mn} \) is the Kronecker function. Clearly,

\[
L_0(x) = 1, \quad L_1(x) = 2x - 1, \quad L_2(x) = 6x^2 - 6x + 1.
\]

Set

\[
S_N = \text{span}\{ L_0(x), L_1(x), \cdots, L_N(x) \}, \quad S^0_N = \{ v \in S_N : v(0) = v(1) = 0 \}.
\]

Denote by \( \langle u, v \rangle \) the inner product of space \( L^2(0,1) \), and by \( \langle u, v \rangle_N \) the corresponding discrete inner product,

\[
\langle u, v \rangle = \int_0^1 u(x)v(x)dx, \quad \langle u, v \rangle_N = \sum_{j=0}^{N} u(x_j)v(x_j)\omega_j,
\]

(2.3)

where \( \{ x_j, \omega_j \}_{j=0}^{N} \) are Legendre-Gauss quadrature nodes and weights.

The Legendre pseudospectral method for (2.2) is to find \( w_N \in S^0_N \otimes S^0_N \) and \( \eta \in \mathbb{R} \) such that

\[
\begin{cases}
\langle \nabla w_N, \nabla \phi \rangle + (\eta + \lambda_0) \langle w_N, \phi \rangle \eta \tau \langle \psi_0, \phi \rangle_N \\
+ k(|x-x| \tau \psi_0 + \tau \psi_0 + \tau \psi_0 + \tau \psi_0), \phi \rangle_N = 0, \\
\langle \psi_0, w_N \rangle = 0, \quad \forall \phi \in S^0_N \otimes S^0_N.
\end{cases}
\]

(2.4)

Next, let

\[
\phi_k(x) = c_k (L_k(x) - L_{k+2}(x)), \quad c_k = \frac{1}{\sqrt{4k+6}}.
\]

Clearly, \( \{ \phi_k(x) \}_{k=0}^{N-2} \) is a set of basis functions of \( S^0_N \). Denote

\[
a_{ij} := \langle \phi_i', \phi_j' \rangle, \quad b_{ij} := \langle \phi_i, \phi_j \rangle.
\]

We deduce readily that

\[
a_{jk} = \begin{cases} 2, & k = j, \\ 0, & k \neq j \end{cases}, \quad b_{jk} = b_{kj} = \begin{cases} c_k c_j \left( \frac{1}{2j+1} + \frac{1}{2j+3} \right), & k = j, \\ -c_k c_j \frac{1}{2k+1}, & k = j + 2, \\ 0, & \text{otherwise.}
\end{cases}
\]

(2.5)
Now, set
\[ \Phi_{ij}(x,y) = \phi_i(x)\phi_j(y). \]

Then \( \{\Phi_{ij}(x,y)\}_{i,j=0}^{N-2} \) is a set of basis functions of \( S_N^0 \otimes S_N^0 \).

We expand the approximate solution as
\[
\begin{aligned}
 w_N(x,y) &= \sum_{i,j=0}^{N-2} w_{ij} \Phi_{ij}(x,y) \\
 &= \sum_{i,j=0}^{N-2} w_{ij} \phi_i(x)\phi_j(y).
\end{aligned}
\]

Let
\[
W = (w_{00}, w_{01}, \cdots, w_{0(N-2)}, \cdots, w_{(N-2)0}, w_{(N-2)1}, \cdots, w_{(N-2)(N-2)})^T,
\]
and take \( \phi(x,y) = \phi_m(x)\phi_n(y) \) in (2.4) for \( 0 \leq m, n \leq N-2 \). Then we find that (2.4) is equivalent to the following matrix equation,
\[
\begin{aligned}
\left\{ \begin{array}{l}
 A \otimes B + B \otimes A + (\eta + \lambda_0) B \otimes B \\
 \langle \psi_0, w_N \rangle_N = 0,
\end{array} \right.
\end{aligned}
\]  
(2.6)

where
\[
\begin{aligned}
 A &= (a_{ij})_{0 \leq i,j \leq N-2}, \\
 B &= (b_{ij})_{0 \leq i,j \leq N-2}, \\
 G &= \eta \tau G_1 + G_2, \\
 G_1 &= \left( \langle \psi_0, \phi_m \phi_n \rangle_N \right)_{0 \leq m,n \leq N-2}, \\
 G_2 &= \left( \langle x|x-x_0|^r |\tau \psi_0 + w_N|^p-1(\tau \psi_0 + w_N), \phi_m \phi_n \rangle_N \right)_{0 \leq m,n \leq N-2}.
\end{aligned}
\]

In actual computations, a Newton-Raphson iterative method is employed to solve the unknowns \( W \) and \( \eta \) of Eq. (2.6) numerically. We can deal with Eq. (1.3) by a similar process.

2.4 Numerical results
In this subsection, we shall compute the multiple solutions of the Schrödinger equation (1.3) by using the suggested algorithm in the last subsection.

2.4.1 Accuracy test of algorithm
To examine the efficiency of our algorithm, we consider the following equation:
\[
\begin{aligned}
\left\{ \begin{array}{l}
 -\Delta u + \lambda u + \kappa |x-x_0|^r |u|^{p-1} u = f(x), \\
 u\big|_{\partial \Omega} = 0.
\end{array} \right.
\]  
(2.7)
\]

For \( f(x) \neq 0 \), Eq. (2.7) admits a unique solution.

Next, let \( \delta u \) be the point-wise numerical errors and take \( \lambda = 1, \kappa = -1, p = 3, r = 1 \). We compute the numerical errors of our algorithm.
(i) Take the exact solution $u(x) = \sin(\pi x_1) \sin(\pi x_2)$, which possesses $D_4$ symmetry. In Fig. 1, we plot the numerical errors $\delta u$ of Legendre pseudospectral method with $N = 20$.

(ii) Take the exact solution $u(x) = \sin(2\pi x_1) \sin(\pi x_2)$, which possesses $\Sigma_1$ symmetry. In Fig. 2, we plot the numerical errors of Legendre pseudospectral method with $N = 20$.

(iii) Take the exact solution $u(x) = \sin(2\pi x_1) \sin(2\pi x_2)$, which possesses $\Sigma_d$ symmetry. In Fig. 3, we plot the numerical errors of Legendre pseudospectral method with $N = 20$.

(iv) Take the exact solution $u(x) = \sin(\pi x_1) \sin(3\pi x_2)$, which possesses $\Sigma_M$ symmetry. In Fig. 4, we plot the numerical errors of Legendre pseudospectral method with $N = 20$. 

Figure 1: The numerical errors of Legendre pseudospectral method.

Figure 2: The numerical errors of Legendre pseudospectral method;
We find that the numerical results of our method are very accurate.

2.4.2 The multiple solutions of (1.3)

In this subsection, we shall compute and visualize the multiple solutions of the Schrödinger equation (1.3), by using Legendre pseudospectral method.

Let \( Rse \) be the residual error of (1.3). In Figs. 5 and 6, we plot the solutions of (1.3) with \( \lambda = 1, \ p = 3, \ k = -1, \ r = 3 \) and various values of \( \lambda_0 \) and \( \psi_0 \). In Figs. 7 and 8, we also plot the solutions of (1.3) with \( \lambda = -100, \ p = 3, \ k = 1, \ r = 3 \) and various \( \lambda_0 \) and \( \psi_0 \). Numerical results show that it is feasible to solve the multiple solutions of the nonlinear problem (1.3) by the bifurcation method. Moreover, we also find that it is not difficult to choose the initial iteration value for obtaining the multiple solutions.
Figure 5: (a) $\lambda_0 = 2 \pi^2$, $\psi_0 = \sin(\pi x_1)\sin(\pi x_2)$, $D_4$ symmetry; (b) $\lambda_0 = 5 \pi^2$, $\psi_0 = \sin(\pi x_1)\sin(2\pi x_2)$, $\Sigma_1$ symmetry; (c) $\lambda_0 = 5 \pi^2$, $\psi_0 = \frac{1}{2} \sqrt{2} (\sin(\pi x_1)\sin(2\pi x_2) + \sin(2\pi x_1)\sin(\pi x_2))$, $\Sigma_2$ symmetry.

Figure 6: (a) $\lambda_0 = 8 \pi^2$, $\psi_0 = \sin(2\pi x_1)\sin(2\pi x_2)$, $\Sigma_4$ symmetry; (b) $\lambda_0 = 10 \pi^2$, $\psi_0 = \frac{1}{2} \sqrt{2} (\sin(\pi x_1)\sin(3\pi x_2) + \sin(3\pi x_1)\sin(\pi x_2))$, $D_4$ symmetry; (c) $\lambda_0 = 13 \pi^2$, $\psi_0 = \sin(2\pi x_1)\sin(3\pi x_2)$, $\Sigma_1$ symmetry.

Figure 7: (a) $\lambda_0 = 2 \pi^2$, $\psi_0 = \sin(\pi x_1)\sin(\pi x_2)$, $D_4$ symmetry; (b) $\lambda_0 = 5 \pi^2$, $\psi_0 = \sin(\pi x_1)\sin(2\pi x_2)$, $\Sigma_1$ symmetry; (c) $\lambda_0 = 5 \pi^2$, $\psi_0 = \frac{1}{2} \sqrt{2} (\sin(\pi x_1)\sin(2\pi x_2) + \sin(2\pi x_1)\sin(\pi x_2))$, $\Sigma_2$ symmetry.
The arclength normalization equation is as follows,

\[ N(u, \lambda; s) := \langle \dot{u}^s, u - \dot{u}^s \rangle + \dot{\lambda}^s (\lambda - \lambda^*) - (s - s^*) = 0, \tag{3.2} \]

where \((u^*, \lambda^*)\) is any given point (in front of fold \((\bar{u}, \bar{\lambda})\)) on the positive solution branch \(\Gamma\) with \(D_4\) symmetry to problem (1.3), and \((\dot{u}^s, \lambda^*)\) is the unit tangent to the branch \(\Gamma\) at

\[ \langle \phi_0, G_\lambda(\bar{u}, \bar{\lambda}, r) \rangle_N \neq 0, \tag{3.1} \]

which means the singular point \((\bar{u}, \bar{\lambda})\) is a simple fold.

To remedy this situation, we use the standard way to reparameterize the problem (1.3) by introducing an approximate arclength parameter \(s\). The arclength normalization equation is as follows,

\[ N(u, \lambda; s) := \langle \dot{u}^s, u - \dot{u}^s \rangle + \dot{\lambda}^s (\lambda - \lambda^*) - (s - s^*) = 0, \tag{3.2} \]

where \((u^*, \lambda^*)\) is any given point (in front of fold \((\bar{u}, \bar{\lambda})\)) on the positive solution branch \(\Gamma\) with \(D_4\) symmetry to problem (1.3), and \((\dot{u}^s, \lambda^*)\) is the unit tangent to the branch \(\Gamma\) at

\[ \langle \phi_0, G_\lambda(\bar{u}, \bar{\lambda}, r) \rangle_N \neq 0, \tag{3.1} \]

which means the singular point \((\bar{u}, \bar{\lambda})\) is a simple fold.

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\[ N(u, \lambda; s) := \langle \dot{u}^s, u - \dot{u}^s \rangle + \dot{\lambda}^s (\lambda - \lambda^*) - (s - s^*) = 0, \tag{3.2} \]

where \((u^*, \lambda^*)\) is any given point (in front of fold \((\bar{u}, \bar{\lambda})\)) on the positive solution branch \(\Gamma\) with \(D_4\) symmetry to problem (1.3), and \((\dot{u}^s, \lambda^*)\) is the unit tangent to the branch \(\Gamma\) at
Therefore \( \dot{\lambda} \) and hence \( \Gamma \) is regular. By Theorem 3.1, we can get the new solution, otherwise the method fails.

**Theorem 3.1.** At the regular points and folds on the positive solution branch \( \Gamma \) with \( D_4 \) symmetry, the Jacobian of Eqs. (1.3) and (3.2)

\[
M(s_0) = \begin{pmatrix}
G^0_u & G^0_\lambda \\
\langle \dot{\lambda}^*, \cdot \rangle & \dot{\lambda}^*
\end{pmatrix}
\]  

is regular.

**Proof.** Differentiating \( G(u(s), \lambda(s), r) = 0 \) with respect to \( s \) at \( s = s_0 \), we get

\[
G^0_u \dot{u}^0 + G^0_\lambda \dot{\lambda}^0 = 0.
\]  

(3.5)

Clearly, if \((u^0, \lambda^0)\) is a regular point on \( \Gamma \), then \( \dot{\lambda}^0 \neq 0 \). Since for \( \dot{\lambda}^0 = 0 \), the regular \( G^0_u \) can lead to \( \dot{u}^0 = 0 \), which is in contradiction with that \((\dot{u}^0, \dot{\lambda}^0)\) is a tangent at \((u^0, \lambda^0)\). Thus, by (3.5) we derive

\[
\frac{\dot{u}^0}{\dot{\lambda}^0} = -(G^0_u)^{-1}G^0_\lambda,
\]

(3.6)

and hence

\[
\dot{\lambda}^* = \langle \dot{\lambda}^*, (G^0_u)^{-1}G^0_\lambda \rangle = \dot{\lambda}^* + \frac{\langle \dot{\lambda}^*, \dot{u}^0 \rangle}{\dot{\lambda}^0} = \frac{1}{\dot{\lambda}^0} (\langle \dot{\lambda}^*, \dot{u}^0 \rangle + \dot{\lambda}^* \dot{\lambda}^0) \neq 0,
\]

(3.7)

which means that \( M(s_0) \) is regular according to the Keller lemma [18, 19].

If \((u^0, \lambda^0)\) is a fold on branch \( \Gamma \), then \( G^0_\lambda \not\in R(G^0_u) \), where \( R(G^0_u) \) is the range of \( G^0_u \). Therefore \( \dot{\lambda}^0 = 0 \) and \( \dot{u}^0 \in N(G^0_u) \), where \( N(G^0_u) \) is the null space of \( G^0_u \). From \( \langle \dot{\lambda}^*, \dot{u}^0 \rangle = \langle \dot{\lambda}^*, \dot{\lambda}^0 \rangle \neq 0 \), we obtain that \( N(\langle \dot{\lambda}^*, \cdot \rangle) \cap N(G^0_u) = \{0\} \), where \( N(\langle \dot{\lambda}^*, \cdot \rangle) \) is the null space of \( \langle \dot{\lambda}^*, \cdot \rangle \). According to the Keller lemma [18, 19], \( M(s_0) \) is regular again.

Theorem 3.1 means that the Newton method can be used to solve problems (1.3) and (3.2), and the pseudo-arclength continuation method may successfully trace the positive solution branch \( \Gamma \) with \( D_4 \) symmetry to problem (1.3) through the fold \((\Pi, \lambda)\). As \( \delta s \) is increased, the solution branch with \( D_4 \) symmetry to problem (1.3) is computed. See Fig. 9(a).
Remark 3.1. In the pseudo-arclength algorithm, \((\dot{u}^*, \dot{\lambda}^*)\) satisfies
\[
\begin{aligned}
G_u \dot{u}^* + G_\lambda \dot{\lambda}^* &= 0, \\
\|\dot{u}^*\|^2 + \|\dot{\lambda}^*\|^2 - 1 &= 0.
\end{aligned}
\] (3.8)
Therefore \(\dot{u}^* = \beta v, \dot{\lambda}^* = \beta\), \(\beta \in \mathbb{R}\), \(v\) satisfies the following problem
\[
\begin{aligned}
-\Delta v + \lambda^* v + p \kappa |x-x_0|^r |u^*|^{p-1} v + u^* &= 0, & x \in \Omega, \\
v|_{\partial \Omega} &= 0,
\end{aligned}
\] (3.9)
and \(\beta = \frac{\pm 1}{\sqrt{1 + \|v\|^2}}\). We must keep the same trend of the solution branch in actual computation. In other word, if \((\dot{u}_{-1}, \dot{\lambda}_{-1})\) is a tangent vector of solution \((u_{-1}, \lambda_{-1})\) (which is in front of the point \((u^*, \lambda^*)\)), we must request \(\beta(\langle \dot{u}_{-1}, v \rangle_N + \dot{\lambda}_{-1}) > 0\). The sign selection of \(\beta\) is very important. If the sign selection is not appropriate, we will not be able to get the new solutions by the pseudo-arclength algorithm.

To determine the fold on the positive solutions with \(D_4\) symmetry, we can use the following extended system:
\[
F(y) = \left( \begin{array}{c} G(u, \lambda, r) \\ G_u(u, \lambda, r) \phi \\ \langle l_0, \phi \rangle_N - 1 \end{array} \right) = 0,
\] (3.10)
where \(y = (u, \phi, \lambda)^T\), \(l_0\) is a normalization of \(\phi\). \(F: Y \rightarrow Y, Y = X^{D_4} \times X^{D_4} \times \mathbb{R}\), \(F\) restricted in \(Y\) is regular.

Remark 3.2. In fact, Eq. (3.10) is the following boundary value problem of PDEs:
\[
\begin{aligned}
-\Delta u + \lambda u + \kappa |x-x_0|^r |u|^{p-1} u &= 0, & x \in \Omega, \\
u|_{\partial \Omega} &= 0, \\
-\Delta \phi + \lambda \phi + p \kappa |x-x_0|^r |u|^{p-1} \phi &= 0, & x \in \Omega, \\
\phi|_{\partial \Omega} &= 0, \\
\phi(\frac{1}{2}, \frac{1}{2}) - 1 &= 0.
\end{aligned}
\] (3.11)
Legendre pseudospectral method is used to discrete Eq. (3.11). The discretized equations of (3.11) can be solved by the Newton method. The initial iteration data \((u_0, \phi_0, \lambda_0)\) may be gotten during continuation. In this paper, we find two folds on the positive solution branch with \(D_4\) symmetry at \(\lambda_1 = 28.7769\) and \(\lambda_2 = 26.6926\). See Fig. 9(a).

3.1.2 The positive solution branch with \(D_4\) symmetry by \(r\) continuation
Taking \(r\) as a parameter, \(\lambda\) as a constant, and using the positive solutions with \(D_4\) symmetry to problem (1.3) with \(r = 0\) as a starting point, we get a whole positive solution...
branch $\Gamma$ with $D_4$ symmetry by $r$ continuation and the Newton method. While $r$ is continued, the eigenvalues of Jacobian $G_u(u,\lambda,r)$ are monitored. We find that the eigenvalues corresponding to small absolute value are near $r = 0.57$ and $2.25$. The corresponding eigenvectors possess $\Sigma_1$, $\Sigma_2$, $\Sigma_M$ and $\Sigma_d$ symmetry, respectively. They are the potential symmetry-breaking bifurcation points [18, 19].

When $r$ is near 12.03, the Newton iteration for problem (1.3) is no longer convergent. There is a singular point $(\bar{u},\bar{r})$ on the positive solution branch with $D_4$ symmetry near $r = 12.03$, where the Jacobian $G_u(\bar{u},\lambda,\bar{r})$ has a zero eigenvalue and the corresponding eigenvector $\phi_0 \in X_{D_4}$. Further calculation shows that
\[ \langle \phi_0, G_r(\bar{u},\lambda,\bar{r}) \rangle_N \neq 0, \quad (3.12) \]
which means the singular point $(\bar{u},\bar{r})$ is a simple fold. We can proceed with the process as in Subsection 3.1.1.

**Remark 3.3.** In the pseudo-arclength algorithm, $(\dot{u}^*,\dot{r}^*)$ satisfies
\[
\begin{align*}
G_u^* \dot{u}^* + G_r^* \dot{r}^* &= 0, \\
\|\dot{u}^*\|^2 + \|\dot{r}^*\|^2 - 1 &= 0.
\end{align*}
\]
Therefore $\dot{u}^* = \beta v$, $\dot{r}^* = \beta$, $\beta \in \mathbb{R}$, $v$ satisfies the following problem
\[
\begin{align*}
-\Delta v + \lambda v + p &\kappa |x-x_0|^{\rho-1}v - \kappa |x-x_0|^{\rho-1}\ln(|x-x_0|)|u^*|^{p-1}u^* = 0, \\
v|_{\partial \Omega} &= 0,
\end{align*}
\]
and $\beta = \frac{\pm 1}{\sqrt{1 + \|v\|^2}}$. We must keep the trend of the solution branch as before. In other word, if $(\dot{u}_{-1},\dot{r}_{-1})$ is a tangent vector of solution $(u_{-1},r_{-1})$ (which is in front of the point $(u^*,r^*)$), we must request $\beta((\dot{u}_{-1},\dot{r}_{-1})_N + \dot{t}_{-1}) > 0$. The sign selection of $\beta$ is very important in the actual computation. If the sign selection is inappropriate, the pseudo-arclength algorithm will not be able to calculate the new solutions.

**Remark 3.4.** To determine the fold on the positive solutions with $D_4$ symmetry, we still use the extended system (3.10). We also find two folds on the positive solution branch with $D_4$ symmetry at $r_1 = 12.0334$ and $r_2 = 11.8514$. See Fig. 10(a).

### 3.2 The symmetry-breaking bifurcation point on the positive solution branch with $D_4$ symmetry

#### 3.2.1 The symmetry-breaking bifurcation point for $\lambda$ continuation

In the following, we take $\lambda$ as a parameter and $r$ as a constant. Let $\Sigma$ be one of $\Sigma_1, \Sigma_2, \Sigma_M, \Sigma_d$, and $X_\Sigma$ be the invariant subspace of $\Sigma$. Since
\[ G(\gamma u,\lambda,r) = \gamma G(u,\lambda,r), \quad \forall \gamma \in D_4, \]
(3.15)
\( X^\Sigma \) can be decomposed into \( X^\Sigma = X^{D_4} \oplus W \), where \( W = X^\Sigma \cap (X^{D_4})^\perp \) and \((X^{D_4})^\perp\) is an orthogonal complement of \( X^{D_4} \).

On the positive solution branch with \( D_4 \) symmetry, there exists a point \((u_0, \lambda_0)\), at which the self-adjoint operator \( G_0^0 = G_u(u_0, \lambda_0, r) \) is singular and its null space is \( \mathcal{N}(G_0^0) = \mathcal{N}(G_0^0)^\perp = \span\{\phi_0\} \) with \( \phi_0 \in W \). If

\[
\langle \phi_0, (G_{u\alpha}^0 p_\lambda + G_{u\lambda}^0) \phi_0 \rangle \neq 0,
\]

(3.16)
and \(v_\lambda \in X^{D_4}\) is the unique solution to
\[
\begin{align*}
G_u^0 v_\lambda + G_\lambda^0 &= 0, \\
\langle \phi_0, v_\lambda \rangle &= 0,
\end{align*}
\]
then the point \((u_0, \lambda_0)\) on the positive solution branch with \(D_4\) symmetry to problem (1.3) is called a \(D_4 - \Sigma\) symmetry-breaking bifurcation point with respect to \(\lambda\).

The following is the extended system for detecting the \(D_4 - \Sigma\) symmetry-breaking bifurcation point:
\[
F(y) = \begin{pmatrix} G(u, \lambda, r) \\ G_u(u, \lambda, r) \phi \\ \langle l_0, \cdot \rangle - 1 \end{pmatrix} = 0,
\]
where \(y = (u, \phi, \lambda)^T \in Y = X^{D_4} \times W \times \mathbb{R}, y_0 = (u_0, \phi_0, \lambda_0), l_0 \in W\) is the normalization of \(\phi\).

**Theorem 3.2.** The extended system (3.18) is regular at the \(D_4 - \Sigma\) symmetry-breaking bifurcation point \(y_0 = (u_0, \phi_0, \lambda_0)\).

**Proof.** Obviously,
\[
F^0_y = \begin{pmatrix} G_u^0 \\ G_u^0 \phi_0 \\ 0 \\ G_\lambda^0 \\ G_u^0 \phi_0 \\ 0 \end{pmatrix}
\]
Next, we prove that \(F^0_y : Y \rightarrow Y\) is one-to-one. To this end, let
\[
F^0_y Z = 0,
\]
where \(Z = (v, w, \alpha)^T, v \in X^{D_4}, w \in W\) and \(\alpha \in \mathbb{R}\). Expanding (3.19) yields
\[
\begin{align*}
G_u^0 v + \alpha G_\lambda^0 &= 0, \\
G_u^0 \phi_0 v + G_\lambda^0 w + \alpha G_u^0 \phi_0 &= 0, \\
\langle l_0, w \rangle &= 0.
\end{align*}
\]
From (3.20), we get \(v = \alpha v_\lambda\). Substituting \(v = \alpha v_\lambda\) into (3.21) and taking the inner product with \(\phi_0\) lead to \(\alpha \langle \phi_0, G_u^0 v_\lambda \phi_0 + G_\lambda^0 \phi_0 \rangle = 0\). Further, by (3.16) we have \(\alpha = 0\). Accordingly, by (3.21) we deduce that \(w = 0\), and thus \(\langle l_0, w \rangle = 0\). We can also prove that \(F^0_y : Y \rightarrow Y\) is onto by a similar argument. Thereby, \(F^0_y\) is regular.

Since \(F^0_y\) is regular, we can use Legendre pseudospectral method to discretize the equations. During the continuation, we use \((u^*, \phi^*, \lambda^*)\) as the initial guess for the Newton iteration process, where \(\phi\) is the corresponding eigenvector of a smaller eigenvalue of Jacobian \(G_u(u, \lambda, r)\). The numerical results are shown in Table 4. From Table 4 we observe that \(\lambda = -7.8499\) and \(\lambda = 24.3012\) are the double symmetry breaking bifurcation points and its null space \(N(G_u(u, \lambda, r)) = \text{span}\{\phi_0^{(1)}, \phi_0^{(2)}\}\) with \(\phi_0^{(1)} \in X^{\Sigma_1}\) and \(\phi_0^{(2)} \in X^{\Sigma_2}\).
Table 4: Symmetry-breaking bifurcation point for \( \lambda \) continuation with \( p = 3, \kappa = -1 \) and \( r = 2 \).

| Table 4: Symmetry-breaking bifurcation point for \( \lambda \) continuation with \( p = 3, \kappa = -1 \) and \( r = 2 \). |
|----|----|----|----|----|----|----|
| \( \lambda \) | \( D_4 - \Sigma_1 \) | \( D_4 - \Sigma_2 \) | \( D_4 - \Sigma_d \) | \( D_4 - \Sigma_M \) | \( D_4 - \Sigma_1 \) | \( D_4 - \Sigma_2 \) |

3.2.2 The symmetry-breaking bifurcation point for \( r \) continuation

In the following, taking \( r \) as a parameter and \( \lambda \) as a constant, we get the symmetry-breaking bifurcation point with respect to \( r \). By using a similar process as in Subsection 3.2.1, we obtain the numerical results shown in Table 5. We also observe that \( r = 0.5688 \) is a double symmetry breaking bifurcation point and its null space \( \mathcal{N}(G_u(u,\lambda,r)) = \text{span} \{ \phi_0^{(1)}, \phi_0^{(2)} \} \) with \( \phi_0^{(1)} \in X^{\Sigma_1} \) and \( \phi_0^{(2)} \in X^{\Sigma_2} \).

Table 5: Symmetry-breaking bifurcation point for \( r \) continuation with \( p = 3, \kappa = -1 \) and \( \lambda = 1 \).

| Table 5: Symmetry-breaking bifurcation point for \( r \) continuation with \( p = 3, \kappa = -1 \) and \( \lambda = 1 \). |
|----|----|----|
| \( r \) | \( D_4 - \Sigma_1 \) symmetry-breaking bifurcation point | \( D_4 - \Sigma_2 \) symmetry-breaking bifurcation point | \( D_4 - \Sigma_d \) symmetry-breaking bifurcation point |
| 0.5688 | 0.5688 | 2.2453 |

3.3 Branch switching to \( \Sigma \) symmetric solutions

3.3.1 Branch switching to \( \Sigma \) symmetric solutions for \( \lambda \) continuation

In the following, we take \( \lambda \) as a parameter and \( r \) as a constant. Let \((\lambda, u)\) be the \( D_4 - \Sigma \) symmetry-breaking bifurcation point with \( \lambda = \lambda_0 \) and \( u = u_0 \in X^{D_4} \), and \( \psi_0 = \phi_0 \in W \). The numerical computation shows

\[
a := \langle \phi_0, G_{u\psi_0}\phi_0 \rangle_N = 0,
b := \langle \phi_0, (G_{u\psi_0}v_\lambda + G_{u\lambda}^0)\phi_0 \rangle_N \neq 0,
c := \langle \phi_0, (G_{u\psi_0}v_\lambda + 2G_{u\lambda}^0v_\lambda + G_{\lambda\lambda}^0)\phi_0 \rangle_N = 0,
\]

where \( v_\lambda \in X^{D_4} \) is the unique solution to Eq. (3.17). By the algebraic bifurcation theory [18, 19], we know that at the symmetry-breaking bifurcation point, tangent vector along the positive solution branch with \( D_4 \) symmetry is \((v_\lambda, 1)\), and tangent vector along the \( \Sigma \) symmetric positive solution branch is \((\phi_0, 0)\). Next, let us define

\[
F(w, \eta, \epsilon) = \begin{cases} 
\epsilon^{-1}G(u_s(\lambda_0 + \eta) + \epsilon(\phi_0 + w), \lambda_0 + \eta, r), & \epsilon \neq 0, \\
G_u(u_s(\lambda_0 + \eta), \lambda_0 + \eta, r)(\phi_0 + w), & \epsilon = 0,
\end{cases} 
\]

\[
N(w, \eta, \epsilon) = \langle \phi_0, w \rangle,
\]

where \( u_s(\lambda) \) is the positive solution with \( D_4 \) symmetry, \( w \in W \) and \( \eta, \epsilon \in \mathbb{R} \). Obviously, \( F(0, 0, 0) = 0 \) and \( N(0, 0, 0) = 0 \). The Jacobian of (3.23) and (3.24) with respect to \( w, \eta \) at
(w,η,ε) = (0,0,0) is that

\[ A^0 = \left. \frac{\partial (F,N)}{\partial (w,\eta)} \right|_{(0,0,0)} = \begin{pmatrix} G_u^0 & B^0 \\ \langle \phi_0, \cdot \rangle & 0 \end{pmatrix}, \]

where

\[ B^0 = \left( G_u^0(u_s(\lambda_0),\lambda_0,r)u'_s(\lambda_0) + G_{u\lambda}^0(u_s(\lambda_0),\lambda_0,r) \right) \phi_0 = \left( G_{uu}^0v_\lambda + G_{u\lambda}^0 \right) \phi_0. \]

Since \( \langle \phi_0, B^0 \rangle = b \neq 0 \) and \( \phi_0 \in \mathcal{N}(G_u^0) \), we have \( B^0 \notin \mathcal{R}(G_u^0) \), \( \mathcal{N}(G_u^0) \cap \mathcal{N}(\langle \phi_0, \cdot \rangle) = \{0\} \). By the Keller lemma \([18, 19]\), \( A^0 \) is nonsingular. The implicit function theorem ensures that the system

\[
\begin{align*}
F(w,\eta,\epsilon) &= 0, \\
N(w,\eta,\epsilon) &= 0
\end{align*}
\]

has a solution \((w(\epsilon), \eta(\epsilon))\) for any \(|\epsilon| < \epsilon_0\), which can be solved by the Newton method. Therefore, we obtain the positive solution branch with \( \Sigma \) symmetry \((u_s(\lambda_0+\eta(\epsilon)) + \epsilon(\phi_0 + w(\epsilon)), \lambda_0+\eta(\epsilon), r)\) to problem (1.3), which is switched from the positive solution branch with \( D_4 \) symmetry.

**Remark 3.5.** During actual computations, we do not need to calculate the second derivative in \( B^0 \), because we always take \( \epsilon \neq 0 \). Problem (3.25) possesses the following form \((p = 3)\):

\[
\begin{align*}
-\Delta w + (\epsilon^2 + \eta + \lambda_0)w - \epsilon^2 u_0(\lambda_0) + (\epsilon^2 + \eta) \left( u_0(\lambda_0) + \epsilon \alpha_2 \psi_0 + \epsilon \beta_2 \nu_\lambda \right) \\
+ \kappa |x - x_0|^\tau \left( 3u_0^2(\lambda_0)w + 3u_0(\lambda_0)(\epsilon \alpha_2 \psi_0 + \epsilon \beta_2 \nu_\lambda + w)^2 + (\epsilon \alpha_2 \psi_0 + \epsilon \beta_2 \nu_\lambda + w)^3 \right) &= 0, \\
\left. w \right|_{\partial \Omega} &= 0, \\
(\alpha_2 \psi_0^T + \beta_2 \nu_\lambda^T) w + \beta_2 \eta &= 0.
\end{align*}
\]

We can solve the above equations by Legendre pseudospectral method with the initial value \((w^0, \eta^0) = (0,0)\). When \( \epsilon \) is big enough, we can get another solution branch. See Fig. 9(b).

**3.3.2** **Branch switching to \( \Sigma \) symmetric solutions for \( r \) continuation**

In the following, we take \( r \) as a parameter and \( \lambda \) as a constant. Let \((u, r)\) be the \( D_4 - \Sigma \) symmetry-breaking bifurcation point with \( r = r_0 \) and \( u = u_0 \in X^{D_4} \), and \( \psi_0 = \phi_0 \in W \). We can get a new positive solution branch by a similar process as in Subsection 3.3.1.
Remark 3.6. The final settlement is the following form \((p = 3)\):

\[
\begin{aligned}
-\Delta w + \lambda w - \epsilon \beta_2 \kappa |x - x_0|^\alpha u_0^3(r_0) \ln |x - x_0| - \kappa| |x - x_0|^\beta_2 + \eta - 1 \\
-3\kappa |x - x_0|^\alpha u_0^3(r_0) \varepsilon (\alpha_2 \psi - \beta_2 v_r) (|x - x_0|^\beta_2 + \eta - 1) \\
+\kappa |x - x_0|^\alpha \varepsilon \beta_2 + \eta \left( 3u_0^2(r_0) w + 3u_0(r_0)(\varepsilon \alpha_2 \psi_0 + \varepsilon \beta_2 v_r + w)^2 \right) \\
+ (\varepsilon \alpha_2 \psi_0 + \varepsilon \beta_2 v_r + w)^3 = 0, \\
w|_{\partial \Omega} = 0, \\
(\alpha_2 \psi^T_0 + \beta_2 v^T_r) w + \beta_2 \eta = 0.
\end{aligned}
\tag{3.26}
\]

We can solve problem (3.26) by Legendre pseudospectral method with the initial value \((u^0, \eta^0) = (0,0)\). When \(\varepsilon\) is big enough, we can also get another solution branch. See Fig. 10(b).

3.4 Numerical results

In Figs. 9(a) and 9(b), we show the \(D_4\) symmetric solution branch to problem (1.3) with \(p = 3, r = 2\) and \(\kappa = -1\), on which there are four symmetry-breaking bifurcation points and two folds for \(\lambda\) continuation. Particularly, we also exhibit in Fig. 9(b) the symmetric positive solutions branching from the symmetry-breaking bifurcation points, which are \(\Sigma_1, \Sigma_2, \Sigma_3, \Sigma_4, \Sigma_5\) and \(D_4\) symmetric, respectively. See lines 1-7. From Fig. 9(b), we further observe that problem (1.3) has only one symmetric positive solution \((D_4)\) for \(-10 < \lambda < -7.8498\), three symmetric positive solutions (resp. \(D_4, \Sigma_1\) and \(\Sigma_2\)) for \(-7.8498 < \lambda < 3.2002\), four symmetric positive solutions (resp. \(D_4, \Sigma_1, \Sigma_2\) and \(\Sigma_4\)) for \(3.2002 < \lambda < 11.6852\), five symmetric positive solutions (resp. \(D_4, \Sigma_1, \Sigma_2, \Sigma_3\) and \(\Sigma_5\)) for \(11.6852 < \lambda < 24.3012\), and seven symmetric positive solutions (resp. \(D_4, \Sigma_1, \Sigma_2, \Sigma_3, \Sigma_4, \Sigma_5\) and \(\Sigma_2\)) for \(24.3012 < \lambda\). The previous seven symmetric positive solutions to problem (1.3) with \(p = 3, r = 2, \kappa = -1, \lambda = 50\) are also plotted in Fig. 11.

In Figs. 10(a) and 10(b), we show the solution branch with \(D_4\) symmetry to problem (1.3) with \(p = 3, \lambda = 1\) and \(\kappa = -1\), on which there are two symmetry-breaking bifurcation points and two folds for \(r\) continuation. Moreover, we also exhibit in Fig. 10(b) the \(\Sigma_1, \Sigma_2\) and \(\Sigma_2\) symmetric positive solutions branching from the symmetry-breaking bifurcation points. In Fig. 10(b) the \(D_4, \Sigma_1, \Sigma_2\) and \(\Sigma_1\) symmetric solution branches are plotted, respectively. From Fig. 10(b), we further observe that problem (1.3) has only one symmetric positive solution \((D_4)\) for \(0 < r < 0.5688\), three symmetric positive solutions (resp. \(D_4, \Sigma_1\) and \(\Sigma_2\)) for \(0.5688361 < r < 2.2453\), four symmetric positive solutions (resp. \(D_4, \Sigma_1, \Sigma_2\) and \(\Sigma_2\)) for \(2.2453 < r\). The previous four symmetric positive solutions to problem (1.3) with \(p = 3, r = 5, \lambda = 1\) and \(\kappa = -1\) are also shown in Fig. 12.
In this paper, we have used Legendre pseudospectral method to compute and visualize the multiple solutions of the Schrödinger equation on a square, based on the Liapunov-Schmidt reduction and symmetry-breaking bifurcation theory. Starting from the non-trivial solution branches of the corresponding nonlinear bifurcation problem, we obtain the multiple solutions of the Schrödinger equation with various symmetries numerically. The bifurcation diagrams are constructed, showing the symmetry/peak phenomena of the Schrödinger equation. Numerical results demonstrate the effectiveness of these approaches.
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