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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.

AMS subject classifications: 35Q55, 35J25, 37M20, 65M70

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

$$\begin{cases} i\dfrac{\partial}{\partial t}w(x,t) = -\Delta w(x,t) + v(x)w(x,t) + \kappa g(x,|w(x,t)|)w(x,t), \\ \dfrac{\partial}{\partial t}\displaystyle\int_{\mathbb{R}^n} |w(x,t)|^2 dx = 0, \end{cases} \tag{1.1}$$

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where $v(x)$ is a potential function, κ 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 $w(x,t)=u(x)e^{i\lambda t}$ are investigated where λ 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):

$$\lambda u(x)=-\Delta u(x)+v(x)u(x)+\kappa g(x,|u(x)|)u(x). \tag{1.2}$$

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

For simplicity, let $v(x)=0$ and λ be a parameter. The aim of this paper is to find the multiple solutions in $H_0^1(\Omega)$ of the following non-autonomous semilinear elliptic PDE:

$$\begin{cases} G(u(x),\lambda,r):=-\Delta u(x)+\lambda u(x)+\kappa|x-x_0|^r|u(x)|^{p-1}u(x)=0, \quad x\in\Omega, \\ u|_{\partial\Omega}=0, \end{cases} \tag{1.3}$$

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

$$J(u)=\int_\Omega\Big[\frac{1}{2}(|\nabla u(x)|^2+\lambda u^2(x))+\frac{\kappa}{p+1}|x-x_0|^r|u(x)|^{p+1}\Big]dx. \tag{1.4}$$

The solutions of (1.3) correspond to the critical points u^* of J, i.e., $J'(u^*)=0$ in $H=H_0^1(\Omega)$. 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 dim $(H^0)<+\infty$. The quantity $\dim(H^-)$ is called the Morse Index (MI) of u^*, and is denoted by MI(u^*). A critical point u^* with MI(u^*)=k ≥ 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 $>k$ ($<k$) 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.