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Spike-Layer Simulation for Steady-State Coupled Schrödinger Equations

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Abstract. An adaptive finite element method is adopted to simulate the steady state coupled Schrödinger equations with a small parameter. We use damped Newton iteration to solve the nonlinear algebraic system. When the solution domain is elliptic, our numerical results with Dirichlet or Neumann boundary conditions are consistent with previous theoretical results. For the dumbbell and circular ring domains with Dirichlet boundary conditions, we obtain some new results that may be compared with future theoretical analysis.

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1. Introduction

Nonlinear Schrödinger equations model a wide range of problems in physics, such as particle movement and Bose-Einstein condensation. If Ω denotes a bounded domain in two-dimensional or three-dimensional space, we consider the following two coupled Schrödinger equations in $H^1(\Omega)\times H^1(\Omega)$:

$$\begin{cases} -\varepsilon^2\triangle u+u=\mu_1u^3+\beta v^2u\,, \\ -\varepsilon^2\triangle v+v=\mu_2v^3+\beta u^2v\,, \\ \quad u,v>0\ in\ \Omega\,, \end{cases} \tag{1.1}$$

subject to either Dirichlet boundary conditions

$$u=v=0\ \ on\ \ \partial\Omega \tag{1.2}$$

or Neumann boundary conditions

$$\frac{\partial u}{\partial n}=\frac{\partial v}{\partial n}=0\ \ on\ \ \partial\Omega\,, \tag{1.3}$$

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where $\triangle = \sum_{i=1}^{N} \partial^2/\partial x_i^2$ is the Laplace operator, Ω is a bounded open domain in $\mathbb{R}^2$ with a smooth boundary $\partial\Omega$, ε is a positive parameter, μ_1 and μ_2 are positive constants, $\beta \in \mathbb{R}$ is also a constant, and n denotes the unit outward normal at $x \in \partial\Omega$. The corresponding energy functional is

$$J_\varepsilon(u,v) = \frac{1}{2}\int_\Omega \left[\varepsilon^2|\nabla u|^2 + u^2 + \varepsilon^2|\nabla v|^2 + v^2\right] dx - \frac{1}{4}\int_\Omega (\mu_1 u^4 + \mu_2 v^4 + 2\beta v^2 u^2)\, dx\,, \quad (1.4)$$

and solutions of the system (1.1) correspond to critical points of J_ε — i.e. $\nabla J_\varepsilon(u,v) = \mathbf{0}$, where ∇J is the Fréchet derivative. Since there is a canonical identification between a Hilbert space and its dual, we always identify the Fréchet derivative with its canonical dual. As in Ref. [4], we consider the Nehari manifold

$$N(\varepsilon,\Omega) = \left\{ \begin{array}{l} (u,v) \in H^1(\Omega)\times H^1(\Omega)\,,\, u \gneqq 0\,,\, v \gneqq 0\,: \\ \displaystyle\int_\Omega \left[\varepsilon^2|\nabla u|^2 + u^2\right] dx = \int_\Omega [\mu_1 u^4 + \beta u^2 v^2]\, dx \\ \displaystyle\int_\Omega \left[\varepsilon^2|\nabla v|^2 + v^2\right] dx = \int_\Omega [\mu_1 v^4 + \beta u^2 v^2]\, dx \end{array} \right\}. \quad (1.5)$$

Any nontrivial positive solution of (1.1) in $H^1(\Omega)\times H^1(\Omega)$ belongs to the manifold (1.5). Among the nontrivial positive solutions, the one or more with the least energy are called the least energy solutions. The least energy solutions of the system (1.1) are minimums of J_ε on $N(\varepsilon,\Omega)$ — i.e.

$$c_\varepsilon = \inf_{(u,v)\in N(\varepsilon,\Omega)} J_\varepsilon(u,v)\,.$$

The system (1.1) arises in the Hartree-Fock theory for a double condensate — i.e. a binary mixture of Bose-Einstein condensates in two different hyperfine states $|1\rangle$ and $|2\rangle$ (cf. Ref. [1]). Physically, u and v are corresponding condensate amplitudes such that $\epsilon^2 = \hbar^2/(2m)$ and $\mu_j = -(N_j - 1)U_{jj}$ where $\hbar$ is the Planck constant, m is the atom mass, and N_j is a fixed number of atoms in the hyperfine state $|j\rangle$. Moreover, we have $N_1, N_2 \geq 1$, $\beta = -N_2 U_{12}$ and $U_{ij} = 4\pi\hbar^2/m\ a_{ij}$, where $a_{jj}\,(j = 1,2)$ and a_{12} are the intraspecies and interspecies scattering lengths. The sign of the scattering length a_{12} determines whether the interactions of states $|1\rangle$ and $|2\rangle$ are repulsive or attractive. When $a_{12} > 0$ (i.e. $\beta < 0$), the interactions of the states $|1\rangle$ and $|2\rangle$ are repulsive, and when $a_{12} < 0$ (i.e. $\beta > 0$) the interactions of the states $|1\rangle$ and $|2\rangle$ are attractive — cf. Ref. [2]. For atoms of the single state $|j\rangle$, when $a_{jj} < 0$ (i.e. $\mu_j > 0$) the interactions of the single state $|j\rangle$ are attractive.

For the case when $\varepsilon = 1\,,\ \Omega = R^2$, there are many contributions on the bound states of the system (1.1). For example, Sirakov [7] discusses when the β problem (1.1) has or has not a least energy solution, and Wang *et al.* [12] construct an unbounded sequence of non-radial positive vector solutions of segregated type in the repulsive case and an unbounded sequence of non-radial positive vector solutions of synchronised type in the attractive case — cf. also Bartsch *et al.* [8] and Lin & Wei [4–6] on the bound states of Schrödinger systems.

When ε is a random positive parameter and Ω is a bounded domain, there are also many articles on the bound states of the system (1.1). Lin & Wei [4] considered the system