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Computing wave functions of nonlinear Schrödinger equations: A time-independent approach

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Abstract

We present a novel algorithm for computing the ground-state and excited-state solutions of M-coupled nonlinear Schrödinger equations (MCNLS). First we transform the MCNLS to the stationary state ones by using separation of variables. The energy level of a quantum particle governed by the Schrödinger eigenvalue problem (SEP) is used as an initial guess to computing their counterpart of a nonlinear Schrödinger equation (NLS). We discretize the system via centered difference approximations. A predictor–corrector continuation method is exploited as an iterative method to trace solution curves and surfaces of the MCNLS, where the chemical potentials are treated as continuation parameters. The wave functions can be easily obtained whenever the solution manifolds are numerically traced. The proposed algorithm has the advantage that it is unnecessary to discretize or integrate the partial derivatives of wave functions. Moreover, the wave functions can be computed for any time scale. Numerical results on the ground-state and excited-state solutions are reported, where the physical properties of the system such as isotropic and nonisotropic trapping potentials, mass conservation constraints, and strong and weak repulsive interactions are considered in our numerical experiments.

Keywords: Bose–Einstein condensates; Gross–Pitaevskii equation; Wave functions; Liapunov–Schmidt reduction; Continuation; Centered difference method; Disk

1. Introduction

In this paper we are concerned with wave functions of M-coupled nonlinear Schrödinger equations (MCNLS), also known as the Gross–Pitaevskii equations (GPE) [35]

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$$\begin{aligned} &\mathrm{i}\frac{\partial}{\partial t}\Phi_j = -\Delta\Phi_j + V_j(x)\Phi_j + \mu_j|\Phi_j|^2\Phi_j + \sum_{i\neq j}\beta_{ij}|\Phi_i|^2\Phi_j \quad \text{for } x\in\mathbf{R}^2,\ t>0,\\ &\Phi_j = \Phi_j(x,t)\in\mathbf{C}, \quad j=1,\ldots,M,\\ &\Phi_j(x,t)\to 0 \quad \text{as } |x|\to+\infty,\ t>0. \end{aligned} \tag{1}$$

Here the solutions Φ_j represent the jth component of the beam in Kerr-like photorefractive media [6], $V_j(x)=\frac{1}{2}(\gamma_{j,1}x_1^2+\gamma_{j,2}x_2^2)$ is the trapping potential with $0\leqslant\gamma_{j,1}\leqslant\gamma_{j,2}$, which is isotropic if $\gamma_{j,1}=\gamma_{j,2}$, otherwise it is called nonisotropic. The coefficients $\mu_j>0$ are for self-defocusing in the jth component of the beam, the coupling constant β_{ij} is the interaction between the ith and the jth components of the beam. The interaction of any two components is attractive if $\beta_{ij}<0$, and repulsive if $\beta_{ij}>0$. Eq. (1) also describes a physical model in which M-species Bose–Einstein condensates (BEC) come from ultra-cold dilute bosonic atoms in a magnetically trapped gas. Experimental reports concerning the BEC can be found, e.g., in [8,9,17,26]. Specifically, Hall et al. [26] reported the first experimental results concerning the dynamics of a two-component system of BEC in the different spin states of ^{87}Rb. For simplicity we denote a single nonlinear Schrödinger equation (NLS) by choosing $M=1$ in Eq. (1).

Eq. (1) has been studied extensively for many years because of their importance in many physical and mathematical problems; see e.g. [5]. Research articles concerning numerical solutions of Eq. (1) can be found, e.g., in [3,11,12,15,32–34,36]. For instance, Muruganandam and Adhikari [34] presented pseudospectral and finite difference methods for the numerical solution of the BEC in three dimensions. Bao and Tang [15] studied the ground-state solution of the BEC by directly minimizing the energy functional. To find the time-dependent solutions of Eq. (1), in general one has to discretize the partial derivatives $\frac{\partial}{\partial t}\Phi_j$, e.g., using the Crank–Nicolson finite difference (CNFD) scheme [2]. Bao et al. [13,14] developed time-splitting spectral approximations for the numerical solutions of Eq. (1), where the Fourier spectral method is used to discretize the Laplacian, and $\frac{\partial}{\partial t}\Phi_j$ are integrated exactly. Recent studies for the numerical solution of the GPE can be found in [23,38,40]. Specifically, Chin and Krotscheck [23] described a fourth-order algorithm for solving the imaginary time GPE in a rotation anisotropic trap. Wang [40] studied the split-step finite difference method for the numerical solution of the NLS.

The purpose of this paper is twofold. First, we wish to indicate that the numerical continuation methods described in [18,20] can be exploited to compute wave functions of Eq. (1). More precisely, let

$$\Phi_j(x,t)=\mathrm{e}^{-\mathrm{i}\lambda_j t}u_j(x), \quad j=1,\ldots,M, \tag{2}$$

where λ_j is the chemical potential, and $u_j(x)$ is a real function independent of time. Then Eq. (1) is transformed into M steady-state coupled NLS of the following form:

$$\begin{aligned} &-\Delta u_j - \lambda_j u_j + V_j(x)u_j + \mu_j u_j^3 + \sum_{i\neq j}\beta_{ij}u_i^2u_j = 0 \quad \text{in } \mathbf{R}^2,\\ &u_j>0 \quad \text{in } \mathbf{R}^2, \quad j=1,\ldots,M,\\ &u_j(x)\to 0 \quad \text{as } |x|\to+\infty. \end{aligned} \tag{3}$$

By the Hartree–Fock theory for BEC, we rewrite Eq. (3) as

$$\begin{aligned} &-\Delta u_j - \lambda_j u_j + V_j(x)u_j + \mu_j u_j^3 + \sum_{i\neq j}\beta_{ij}u_i^2u_j = 0 \quad \text{in } \Omega, \quad j=1,\ldots,M,\\ &u_1=u_2=\cdots=u_M=0 \quad \text{on } \partial\Omega. \end{aligned} \tag{4}$$

To be consistent with the physical meaning of Eq. (1), we assume that Ω is the unit disk in $\mathbf{R}^2$, see e.g. [27]. Eq. (4) is a nonlinear system of M equations of the following form:

$$F_j(u_1,\ldots,u_M,\lambda_j,\mu_j,\beta_{1j},\ldots,\beta_{j-1,j},\beta_{j+1,j},\ldots,\beta_{Mj})=0, \quad j=1,\ldots,M, \tag{5}$$

where F_j: $B_1\times\mathbf{R}^{M+1}\to B_2$ and $F(\cdot)=(F_1(\cdot),\ldots,F_M(\cdot))$, and B_1 and B_2 are two Banach spaces. For simplicity we keep the coefficients of the cubic terms fixed, and denote a point on the solution manifolds of Eq. (5) by $\{(u_j,\lambda_j)\}_{j=1:M}$. For $M=3$ Eq. (4) can be expressed as