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On numerical methods for nonlinear singularly perturbed Schrödinger problems

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Abstract

Nonlinear Schrödinger equations (NSE) model several important problems in Quantum Physics and Morphogenesis. In case of singularly perturbed problems, the theory have made interesting progress, but numerical methods have been not able to come up with small values of the singular parameter ε. Moreover, the saddle-point characteristic of the associated functional is another challenge that it was first studied by Choi & McKenna, who developed the Mountain Pass Algorithm. We will focus on NSE where a uniqueness result for ground-state solutions is obtained. In this article, we develop a new method which improves the results for a large range of singular parameters. We extend the MPA ideas considering the singulary perturbed problems by developing a finite element approach mixed with steepest descend directions. We use a modified line search method based on Armijo's rule for improving the Newton search and Patankar trick for preserving the positiveness of the solution. To improve the range of the singular parameter, adaptive methods based on Dual Weighted Residual method are used. Our numerical experiments are performed with the deal.II library and we show that it is possible to get solutions for $\varepsilon = 10^{-6}$ improving the current results in four order of magnitude. At this level, machine precision must be considered for further studies.

Keywords: singularly perturbed Schrödinger problems, Mountain Pass Algorithm, Patankar trick, dual weighted residual method

Mathematics subject classifications (1991): 35Q55, 65N30, 65N50

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