Computing the ground state and dynamics of the nonlinear Schrödinger equation with nonlocal interactions via the nonuniform FFT

Weizhu Bao\textsuperscript{a}, Shidong Jiang\textsuperscript{b}, Qinglin Tang\textsuperscript{c,d}, Yong Zhang\textsuperscript{e,f,}\textsuperscript{*}

\textsuperscript{a}Department of Mathematics, National University of Singapore, Singapore 119076, Singapore
\textsuperscript{b}Department of Mathematical Sciences, New Jersey Institute of Technology, Newark, New Jersey, 07102, USA
\textsuperscript{c}Université de Lorraine, Institut Elie Cartan de Lorraine, UMR 7502, Vandoeuvre-lès-Nancy, F-54506, France
\textsuperscript{d}Inria Nancy Grand-Est/IECL-CORIDA, France
\textsuperscript{e}Wolfgang Pauli Institute c/o Fak. Mathematik, University Wien, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria
\textsuperscript{f}Beijing Computational Science Research Center, Beijing 100084, P. R. China

Abstract

We present efficient and accurate numerical methods for computing the ground state and dynamics of the nonlinear Schrödinger equation (NLSE) with nonlocal interactions based on a fast and accurate evaluation of the long-range interactions via the nonuniform fast Fourier transform (NUFFT). We begin with a review of the fast and accurate NUFFT based method in [29] for nonlocal interactions where the singularity of the Fourier symbol of the interaction kernel at the origin can be canceled by switching to spherical or polar coordinates. We then extend the method to compute other nonlocal interactions whose Fourier symbols have stronger singularity at the origin that cannot be canceled by the coordinate transform. Many of these interactions do not decay at infinity in the physical space, which adds another layer of complexity since it is more difficult to impose the correct artificial boundary conditions for the truncated bounded computational domain. The performance of our method against other existing methods is illustrated numerically, with particular attention on the effect of the size of the computational domain in the physical space. Finally, to study the ground state and dynamics of the NLSE, we propose efficient and accurate numerical methods by combining the NUFFT method for potential evaluation with the normalized gradient flow using backward Euler Fourier pseudospectral discretization and time-splitting Fourier pseudospectral method, respectively. Extensive numerical comparisons are carried out between these methods and other existing methods for computing the ground state and dynamics of the NLSE with various nonlocal interactions. Numerical results show that our scheme performs much better than those existing methods in terms of both accuracy and efficiency.

Keywords: nonlinear Schrödinger equation, nonlocal interactions, nonuniform FFT, ground state, dynamics, Poisson equation, fractional Poisson equation

1. Introduction

In this paper, we present efficient and accurate numerical methods and compare them with existing numerical methods for computing the ground state and dynamics of the nonlinear Schrödinger equation (NLSE). In dimensionless form, the NLSE with a nonlocal (long-range) interaction in $d$-dimensions ($d$ =

\textsuperscript{*}Corresponding author.

\textit{Email addresses:} matbaowz@nus.edu.sg (Weizhu Bao), shidong.jiang@njit.edu (Shidong Jiang), qinglin.tang@inria.fr (Qinglin Tang), yong.zhang@univie.ac.at (Yong Zhang)

\textit{URL:} http://www.math.nus.edu.sg/~bao/ (Weizhu Bao)