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## An adaptive Galerkin method for the time-dependent complex Schrödinger equation \*

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### Abstract

Nonlinear time-dependent Schrödinger equations (NLSE) model several important problems in quantum physics and morphogenesis. Recently, vortex lattice formation were experimentally found in Bose-Einstein condensate and Fermi superfluids, which are modeled by adding a rotational term in the NLSE equation. Numerical solutions have been computed by using separate approaches for time and space variables. If we see the complex equation as a system, wave methods can be used. In this article, we consider finite element approximations using continuous Galerkin schemes in time and space by adaptive mesh balancing both errors. To get this balance, we adapt the dual weighted residual method used for wave equations and estimates of error indicators for adaptive space-time finite element discretization. The results show how important is dynamic refinement to control the degrees of freedom in space.

**Key words:** nonlinear time-dependent Schrödinger equation, dual weighted residual method, adaptive Galerkin method

**Mathematics subject classifications (2000):** 35B40, 35P30, 35Q55, 65N25, 81Q05.

### References

- [1] G.D. AKRIVIS, V.A. DOUGALIS, AND O.A. KARAKASHIAN, *On fully discrete Galerkin methods of second order temporal accuracy for the nonlinear Schrödinger equation*. Numer. Math., 59 (1991), no. 1, 31–54.

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- [2] M.H. ANDERSON, J.R. ENSHER, M.R. MATTHEWS, C.E. WIEMAN, AND E.A. CORNELL, *Observation of Bose-Einstein condensation in a dilute atomic vapor*. Science 269 (1995), no. 5221, 198–201.
- [3] X. ANTOINE AND R. DUBOSCQ, *Robust and efficient preconditioned Krylov spectral solvers for computing the ground states of fast rotating and strongly interacting Bose-Einstein condensates*, J. Comput. Phys. 258 (2014), 509–523.
- [4] A.I. AVILA, A. MEISTER, AND M. STEIGEMANN, *On numerical methods for nonlinear singularly perturbed Schrödinger problems*. Appl. Num. Math. 86 (2014), 22–42.
- [5] W. BANGERTH, M. GEIGER, AND R. RANNACHER, *Adaptive Galerkin finite element methods for the wave equation*- Comp. Meth. Appl. Math. 10 (2010), no. 1, 3–48.
- [6] W. BANGERTH, R. HARTMANN, AND G. KANSCHAT, *deal.II: a general-purpose object-oriented finite element library*. ACM Trans. Math. Softw. 33 (2007), no. 4, 4.
- [7] W. BANGERTH AND R. RANNACHER, *Adaptive finite element methods for differential equations*. Lectures in Mathematics, Birkhäuser Verlag, Basel, Boston, Berlin, 2003.
- [8] W. BAO AND Y. CAI, *Mathematical theory and numerical methods for Bose-Einstein condensation*. Kinet. Relat. Mod. 6 (2013), no. 1, 1–135.
- [9] W. BAO, H. WANG, AND P. A. MARKOWICH, *Ground, symmetric and central vortex states in rotating Bose-Einstein condensates*. Comm. Math. Sci. 3 (2005), no. 1, 57–88.
- [10] R. BECKER AND R. RANNACHER, *A feed-back approach to error control in finite element methods: basic analysis and examples*. East-West J. Numer. Math. 4 (1996), 237–264.
- [11] R. BECKER AND R. RANNACHER, *An optimal control approach to a posteriori error estimation in finite element methods*. Acta Numerica 2001 10 (2001), 1–102.
- [12] M. BESIER AND R. RANNACHER, *Goal-oriented space-time adaptivity in the finite element Galerkin method for the computation of nonstationary incompressible flow*. Int. J. Numer. Meth. Fluids (2011), 1–29.
- [13] I. BLOCH, J. DALIBARD, AND W. ZWERGER, *Many-body physics with ultracold gases*. Rev. Mod. Phys. 80 (2008), no. 3, 885–944.
- [14] K. ERIKSSON, D. ESTEP, AND C. HANSBO, P. JOHNSON, *Computational differential equations*. Cambridge University Press, 1996.
- [15] E. HAIRER, C. LUBICH, AND G. WANNER, *Geometric numerical integration*. Series in Computational Mathematics, vol. 31, Springer, Berlin, Heidelberg, 2002.
- [16] P. HENNING AND A. MALQVIST, *The finite element method for the instationary Gross-Pitaevskii equation with angular momentum rotation*. arXiv:1502.05025v2 (2015), 1–30.

- [17] H. HOFSTÄTTER, O. KOCH, AND M. THALHAMMER, *Convergence analysis of high-order time-splitting pseudo-spectral methods for rotational Gross-Pitaevskii equations.* Numer. Math. 127 (2014), 315–364.
- [18] J. MING, Q. TANG, AND Y. ZHANG, *An efficient spectral method for computing dynamics of rotating two-component Bose-Einstein condensates via coordinate transformation.* J. Comput. Phys. 258 (2014), no. 1, 538–554.
- [19] M. SCHMICH AND B. VEXLER, *Adaptivity with dynamic meshes for space-time finite element discretizations of parabolic equations.* SIAM J. Sci. Comput. 30 (2008), no. 1, 369–393.
- [20] J. WLOKA, *Partial differential equations.* Cambridge University Press, 1987.
- [21] M.W. ZWIERLEIN, J.R. ABO-SHEER, A. SCHIROTZEK, C.H. SCHUNCK, AND W. KETTERLE, *Vortices and superfluidity in a strongly interacting Fermi gas.* Nature 435 (2005), 1047–1051.