# Adaptive High-order Splitting Methods for Schrödinger Equations

Othmar Koch (Vienna University of Technology)

W. Auzinger, H. Hofstätter (Vienna University of Technology), and M. Thalhammer (University of Innsbruck)

We discuss the time integration of nonlinear Schrödinger equations by high-order splitting methods. The convergence is analyzed first for the semi-discretization in a general Banach space framework [3]. For the Gross-Pitaevskii equation with rotation term, a generalized Laguerre–Fourier–Hermite method is employed for the full discretization. The convergence of this method is established theoretically and illustrated by numerical examples [2]. To obtain efficient integrators, adaptive time-stepping is introduced. As a basis, two classes of local error estimators based on embedded pairs of splitting formulae [4] and the defect correction principle [1] are put forward and their asymptotical correctness is demonstrated.

## References

[1] W. Auzinger, O. Koch, and M. Thalhammer, Defect-based local error estimators for splitting methods, with application to Schrödinger equations, Part I. The linear case. *J. Comput. Appl. Math. 236(10)*, pp. 2643–2659 (2012).

[2] H. Hofstätter, O. Koch, and M. Thalhammer, Convergence of split-step generalized-Laguerre–Fourier–Hermite methods for Gross–Pitaevskii equations with rotation term. Submitted to Numer. Math. Preprint available from `http://www.asc.tuwien.ac.at/preprint/2012/asc32x2012.pdf`

[3] O. Koch, Ch. Neuhauser, and M. Thalhammer, Error analysis of high-order splitting methods for nonlinear evolutionary Schrödinger equations and application to the MCTDHF equations in electron dynamics. *to appear in M2AN Math. Model. Numer. Anal.*.

[4] O. Koch, Ch. Neuhauser, and M. Thalhammer, Embedded split-step formulae for the time integration of nonlinear evolution equations. *Appl. Numer. Math. 63* (2013), pp. 14–24.