Adaptive Magnus-type integrators for the simulation of solar cells

Othmar Koch

joint with W. Auzinger, H. Hofstätter, M. Quell, and M. Thalhammer

April 12, 2018

We present adaptive time integrators for large systems of linear homogeneous Schrödinger-type ODEs

$$\mathrm{i}\dot{\psi}(t) = H(t)\psi(t),$$

with an Hermitian matrix $H(t)$, which results from spatial discretization for example based on Wannier functions. One motivation for studying such systems is the simulation of novel oxide solar cells which promise gains in the efficiency of energy conversion. A favorable approach for the numerical solution of such problems is given by commutator-free Magnus-type methods. The oscillatory and rapidly attenuating electric field caused by the impact of a photon and almost stationary behavior thereafter call for adaptive choice of the time-steps. To this end, several approaches for the estimation of the local error are promising. A defect-based error estimator is constructed and its asymptotical correctness is proven [1], and additionally a simple mechanism to increase the accuracy of the error estimator for symmetric time integrators is introduced [2]. Moreover, optimal methods are constructed which can be endowed with embedded error estimators. In each step, the Lanczos method is employed for the task of matrix exponentiation. We also show that the eigenvalues of $H(t)$ are independent of time, which implies that time-steps for the Lanczos method can be chosen as uniform.

References

[1] W. Auzinger, H. Hofstätter, O. Koch, M. Quell, and M. Thalhammer, *A posteriori error estimation for Magnus-type integrators*, submitted. Preprint at `http://www.asc.tuwien.ac.at/preprint/2018/asc01x2018.pdf`.

[2] W. Auzinger and O. Koch, *An improved local error estimator for symmetric time-stepping schemes*, Appl. Math. Lett. 82(2018), pp.106-110. Archived at `https://uscholar.univie.ac.at/view/o:717623`.