

# Numerical Analysis Seminar in SS 2009 on "Numerical Methods in Quantum Molecular Dynamics"

## **Topics**

(roman numbers refer to sections in [6])

- 1) Introduction: Quantum vs. Classical Dynamics (I)

### *Model Reduction*

- 2) The Dirac-Frenkel Time-Dependent Variational Principle and Quasi-Optimality of Variational Approximations (II.1 and II.6)
- 3) Adiabatic / BornOppenheimer Approximation (II.2)
- 4) Self-Consistent Field Methods (II.3)
- 5) Parametrized Wave Functions and Mixed Models (II.4 and II.5)

### *Numerical Methods*

- 6) Space Discretization by Spectral Methods: Hermite (III.1.1 and III.1.2 with implementations and examples)
- 7) Space Discretization by Spectral Methods: Fourier (III.1.3 and III.1.4 with implementations and examples)
- 8) Polynomial Approximations to the Matrix Exponential: (III.2.2 and [4, 3, 7] with implementation and examples)

- 9) Splitting and Composition Methods (III.3)
- 10) Integrators for Time-Dependent Hamiltonians (III.4 and [5, 1])
- 11) Variational Space Discretization (IV.1)
- 12) Variational Splitting (IV.2 and IV.3)
- 13) Variational Splitting for Gaussian Wave Packets (IV.4 and [2] and implementation)

## References

- [1] S. Blanes, P.C. Moan, *Splitting methods for the time-dependent Schrödinger equation*. Physics Letters A 265 (2000), 35–42
- [2] E. Faou, C. Lubich, *A Poisson integrator for Gaussian wavepacket dynamics*. Comput. Vis. Sci. 9 (2006), 45–55.
- [3] N. J. Higham, *Functions of matrices*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2008.
- [4] M. Hochbruck, C. Lubich, *On Krylov subspace approximations to the matrix exponential operator*. SIAM J. Numer. Anal. 34 (1997), 1911–1925.
- [5] M. Hochbruck, C. Lubich, *On Magnus integrators for time-dependent Schrödinger equations*. SIAM J. Numer. Anal. 41 (2003), 945–963.
- [6] C. Lubich, *From Quantum to Classical Molecular Dynamics: Reduced Models and Numerical Analysis*. Europ. Math. Soc., Zürich, 2008. This book is available from Vasile Gradinaru ([vasile.gradinaru@sam.math.ethz.ch](mailto:vasile.gradinaru@sam.math.ethz.ch)).
- [7] T.J. Park, J.C. Light, *Unitary quantum time evolution by iterative Lanczos reduction*. J. Chem. Phys. 85 (1986), 5870–5876.