Preface

> For dealing with atoms involving many electrons the accurate quantum theory, involving a solution of the wave equation in many-dimensional space, is far too complicated to be practicable. One must therefore resort to approximate methods. (P.A.M. Dirac, 1930)

This book is not about Nature, but about tools for exploring Nature. It is written by a mathematician who does not himself apply these tools but who appreciates their uses, admires their shapes, analyses their function, and at times designs improved hand axes.

Quantum dynamics of molecules poses a variety of computational challenges that are presently at the forefront of research efforts in numerical analysis in a number of application areas: high-dimensional partial differential equations, multiple scales, highly oscillatory solutions, and geometric structures such as symplecticity and reversibility that are favourably preserved in discretizations. This text addresses such problems in quantum mechanics from the viewpoint of numerical analysis, illustrating them to a large extent on intermediate models between the Schrödinger equation of full many-body quantum dynamics and the Newtonian equations of classical molecular dynamics. The fruitful interplay between quantum dynamics and numerical analysis is emphasized: numerical algorithms originally developed for quantum dynamics sometimes find a much wider scope of application areas, and numerical analysis can contribute theoretical hindsight and novel algorithms to computational quantum dynamics.

This short book contains the extended lecture notes of a graduate course (Nachdiplomvorlesung) held at ETH Zürich in the winter semester 2007. It has five chapters: Chapter I gives a concise introduction to quantum mechanics and establishes basic notions and notation. Chapter II treats the Dirac–Frenkel time-dependent variational principle and reduced models for many-body quantum dynamics built on it. Numerical methods for linear time-dependent Schrödinger equations are studied in Chapter III, those for the non-linear equations of motion of reduced models in Chapter IV. Finally, Chapter V describes a novel numerical approach to the Schrödinger equation in semi-classical scaling, using Hagedorn wave packets. The selection of topics has been guided by the wish to include a wide variety of beautiful ideas and successful techniques, with no attempt at encyclopedic completeness.

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