Preface

Since 1983 I have been delivering lectures at Budapest University that are mainly attended by chemistry students who have already studied quantum chemistry in the amount required by the (undergraduate) chemistry curriculum of the University, and wish to acquire deeper insight in the field, possibly in preparation of a master's or Ph.D. thesis in theoretical chemistry. In such a situation, I have the freedom to discuss, in detail, a limited number of topics which I feel are important for one reason or another. The exact coverage may vary from year to year, but I usually concentrate on the general principles and theorems and other basic theoretical results which I foresee will retain their importance despite the rapid development of quantum chemistry.

I commonly organize my lectures by treating the subject from the beginning, without referring explicitly to any actual previous knowledge in quantum chemistry—only some familiarity with its goals, approaches and, to a lesser extent, techniques is supposed. I concentrate on the formulae and their derivation, assuming the audience essentially understands the reasons for deriving these results.

This book is basically derived from the material of my lectures. The special feature, distinguishing it from most other textbooks, is that all results are explicitly proved or derived, and the derivations are presented completely, step by step. True understanding of a theoretical result can be achieved only if one has gone through its derivation.

Accordingly, this book may be considered a textbook "from the beginning but not for beginners." This means that to fully understand the book, only a familiarity with the simplest notions of quantum mechanics are required. These notions are the concepts of wave functions, operators and their matrix elements, the time-dependent and time-independent Schrödinger equation, as well as some basic knowledge of calculus, linear and matrix algebra. Any material which I suppose that may be absent from a chemist's curriculum is included either in the text or in an appendix. Therefore, anybody to whom the

book appears to be of interest based upon its title should have the necessary knowledge to read it. The book, however, is not intended as a first introduction to quantum chemistry (except, possibly, for a professional physicist); much emphasis is put on the formulae and their derivation and little on their practical utilization. (For these practical aspects I can recommend studying Veszprémi and Fehér's *Quantum Chemistry*, Kluwer Academic/Plenum Publishers 1999.) Thus, despite the limited amount of knowledge assumed, the book does not represent very easy reading: it requires the ability to follow the (sometimes-not-so-short) derivations and proofs. I think the title of the book reflects these aspects—relative simplicity and the emphasis put on formalism.

The book contains many results supposed to be familiar to professionals working in the field, but not included in introductory textbooks. At the same time, it may be rather difficult to find sources containing detailed derivations or proofs of these "commonplaces," especially such derivations which do not use a more refined formalism, e.g., second quantization. No second quantization, no density matrices, no diagrams and practically no group theory are used in this book, so it is also suited well to the needs of those who have their background in chemistry, rather than in theoretical physics.

Whereas the book is mainly intended for future professionals (students and young specialists) in theoretical chemistry and related fields (spectroscopy, material research, molecular physics etc.) I hope my fellow quantum chemists and molecular physicists will also find the book a useful source of simple proofs and derivations when they prepare their lectures.

The material in the book is presented as simply as possible. The treatment remains at the so-called "physical level of rigor". I did not follow the conventional presentation if I could develop a better one. In particular, I treat all the variational problems based on the same equivalent reformulation of the variation principle Eq.(2.13), which leads, for instance, to a very simple derivation of the Hartree-Fock equations via the Brillouin theorem. (However, in some cases the alternative derivations by using the Lagrangian multiplier technique are also shown for completeness.)

The book is self-contained and for the most part avoids questions of priority. Therefore it does not contain extensive literature surveys, only short bibliographical notes quoting some basic references and giving credit to the sources where I have learned some non-standard material.

Last, but not least, I should express my gratitude to my colleague Dr. Andrea Hamza who has read the entire manuscript and made substantial contributions to its improvement, I also thank Professor Péter R. Surján, Professor Dalia Satkovskiene, Dr. Imre Pápai and Dr. Gábor Schubert for their useful comments on some parts of the manuscript. The preparation of the manuscript has been done, for the most part, by Zsuzsa Kertész. I am indebted to her for her meticulous work in placing the bulky formulae into LaTeX.