

Preface

This book emerged from a course on density functional theory (DFT), first given at the University of Munich more than a decade ago. The course was based on the classic texts by Dreizler and Gross (Springer, 1990) and by Parr and Yang (Oxford University Press, 1989). More recent topics of that time, such as time-dependent DFT or orbital-dependent functionals, were added to the material covered by the two books. However, already at that time restriction to the most relevant and/or most illustrative statements on a particular aspect of DFT was necessary, in order to keep the length of the course under control. When the course was later given again at the University of Frankfurt it soon turned out to be impossible to integrate the exploding number of new results, concerning both the formalism as well as important applications, into the course: So, even a selection of the branches of DFT covered in the course was unavoidable.

The present text reflects this, admittedly subjective, choice of topics: it concentrates on the basics of the most widely used variants of DFT. This implies a thorough discussion of the corresponding existence theorems and effective single-particle equations as well as of the key approximations utilized in implementations. Ground state DFT (on the nonrelativistic level) is addressed in Chaps. 2–6. Chapter 2 introduces the fundamental Hohenberg-Kohn theorem and its extensions to spin-, current- and current-spin-density functional theory, together with some basic notions such as v -representability. The resulting Kohn-Sham equations are collected in Chap. 3. This chapter also includes a discussion of the relation between the Kohn-Sham wavefunctions and eigenvalues and the true many-body wavefunctions and energies. Chapter 4 is devoted to a detailed exposition of the currently available approximations for the exchange-correlation functional, based on two exact representations of this quantity. The most important virial relations valid for density functionals are summarized in Chap. 5. The discussion of the exchange-correlation functional is then resumed in Chap. 6, in which the concept of orbital-dependent functionals is introduced. This chapter also serves as a demonstration of the first-principles character of DFT, in that it shows that the true exchange-correlation energies and potentials can be systematically approached by use of orbital-dependent functionals. On the other hand, the discussion of the existence theorem, of the basic

formalism and of standard approximations is concentrated in a single chapter in the case of time-dependent DFT (Chap. 7). The same statement applies to relativistic DFT which is presented in Chap. 8. An extended review of the problem of renormalization (in the Appendices F–I) serves as background information for relativistic DFT.

Throughout the text formal statements are complemented by selected quantitative results, which primarily aim at an illustration of the strengths and weaknesses of a particular approach or functional. However, no attempt is made to review the full range of present-day DFT applications, not even their boundaries will be marked out. In order to stay within reasonable bounds, the discussion also omits a few topics which have recently attracted much interest, such as DFT for superconducting or hadronic systems. An overview of the topics not covered explicitly in this book is provided by Chap. 9 (*Further Reading*) which offers a substantial collection of pertinent papers together with some comments.

The students in the courses indicated above had quite diverse backgrounds, ranging from mineralogy to biochemistry. So, the courses had to be rather self-contained, requiring neither the audience's familiarity with standard many-body theory nor extensive experience with the quantum theory of solids. Again, the book reflects this fact: the reader will find that all concepts of many-body theory which are indispensable for the discussion of DFT, such as the single-particle Green's function or response functions, are introduced step by step, rather than just used. The same applies to some basic notions of solid state theory, as, for instance, the Fermi surface. In fact, even the language of second quantization is introduced systematically in an Appendix. When starting with this Appendix, reading this book should require little more than a strong background in elementary quantum mechanics (at least, if one accepts some of the more advanced relations of Chap. 4 without going through their derivations¹).

As is clear from these remarks, this book does not target only one particular scientific community. On the other hand, the material is easily restricted to the needs of a more specialized course. Many of the advanced chapters require little more than knowledge of the most elementary parts of the introductory chapters. Several redundancies help to support this modular structure. It should therefore be possible to find one's own way through the material. Although detailed recommendations have obvious problems, some suggestions for selected reading are made in the following table:

¹ An alternative, low level entry point to the discussion of the exchange-correlation energy functional is provided by Appendix D, in which the local density approximation for the exchange functional is derived explicitly without using concepts from many-body theory. With the background of this appendix it should be possible to continue with the more advanced results and explicit functionals of Chap. 4.