

Preface to the Second Edition

The idea of writing a second edition within slightly more than a decade of the publication of the first is a consequence of the considerable new understandings of Quantal Density Functional Theory (Q-DFT) achieved over this period. But there have also been further insights into Schrödinger theory, and to the significance of the first theorems of Hohenberg-Kohn and Runge-Gross density functional theory (DFT). The book is still comprised of the three principal components: a description of Schrödinger theory from the new perspective of the ‘Quantal Newtonian’ second and first laws for the individual electron; traditional Hohenberg-Kohn, Runge-Gross, and Kohn-Sham density functional theory; and Q-DFT together with applications to explicate the theory, and the physical insights it provides into traditional DFT, Slater theory, and local effective potential energy theory in general. However, each component has been revised to incorporate the new understandings. Then there is the new material on the extension of Q-DFT to the added presence of an external magnetostatic field. It was the attempt to extend the theory to the presence of magnetic fields that forced the reexamination of both traditional DFT and Q-DFT, thereby leading to many of the new insights. The extension to external magnetic fields required a critical reevaluation of the existing literature. This in turn led to the proof of the corresponding Hohenberg-Kohn theorems for uniform magnetostatic fields, one that is distinct from but in the rigorous sense of the original. The Q-DFT in a magnetic field is then explicated by an example in two-dimensional space. Working on the second edition has been akin to writing a new book.

The pedagogical nature of the book has been maintained. Most of the new derivations are once again given in detail. And as a result of the new understandings, it has been possible to present Q-DFT for arbitrary external electromagnetic fields whether they be time-dependent or time-independent in a most general and comprehensive manner. The common thread of the ‘Quantal Newtonian’ laws for the individual electron is now weaved throughout the book.

Xiaoyn Pan has been a principal contributor to the new developments. Our collaboration has been productive, and working with Xiaoyin has been a pleasure.

Together with Doug Achan, a former graduate student, and Lou Massa, a friend and colleague, new physics of the Wigner low-density high-electron correlation regime of a nonuniform density system has been discovered. Thus, an additional characterization of the Wigner regime is proposed. The example studied also provides a contrast to the high-density low-electron correlation regime of atoms and molecules.

Thanks are also due to Xiaoyin and Lou for their critical comments on various chapters.

Once again I wish to acknowledge Brooklyn College for the support and freedom afforded to me to pursue the research of my interest.

Finally, with much gratitude, I wish to thank my wife Catherine for typing the book despite the travails of life.

Brooklyn, NY, USA

Viraht Sahni

Preface to the First Edition

The idea underlying this book is to introduce the reader to a new local effective potential energy theory of electronic structure that I refer to as Quantal Density Functional Theory (Q-DFT). It is addressed to graduate students who have had a one year course on Quantum Mechanics, and to researchers in the field of electronic structure. It is pedagogical, with detailed proofs, and many figures to explain the physics. The theory is based on the first Hohenberg–Kohn theorem, and is distinct from Kohn–Sham density functional theory. No prior understanding of traditional density functional theory is required as the theorems of Hohenberg and Kohn, and Kohn–Sham theory, and their extension to time-dependent phenomenon are described. There are other excellent texts on traditional density functional theory, and as such I have kept the overlap with the material in these texts to a minimum. It is also possible via Q-DFT to provide a rigorous physical interpretation of Kohn–Sham theory and other local effective potential energy theories such as Slater theory and the Optimized Potential Method. A second component to the book is therefore the description and the explanation of the physics of these theories.

My interest in density functional theory began in the early 1970s simultaneously with my work on metal surface physics. The origins of Q-DFT thus lie in my attempts to understand the physics underlying the formal framework of Kohn–Sham density functional theory and of various approximations within it in the context of the nonuniform electron gas at a metal surface. My work with Manoj Harbola [1, 2] constitutes the ideas seminal to Q-DFT. The history of how these ideas developed, and of their evolution to Q-DFT, is a classic example of how science works. This is not the place to describe the many twists and turns in the path to the final version of the theory. However, together with a further understanding [3] noted, credit must also be afforded Andrew Holas and Norman March whose work [4] helped congeal and close the circle of ideas.

I wish to gratefully acknowledge my graduate students Cheng Quinn Ma, Abdel Mohammed, Manoj Harbola, Marlina Slamet, Alexander Solomatin, Zhixin Qian, and Xiaoyin Pan whose creative work has contributed both directly and indirectly to the writing of this book.

Then there is my friend and colleague Lou Massa whose enthusiasm for the subject matter of the book and whose consistent support and critique during its writing have proved invaluable.

Brooklyn College has been home, and I thank the College for its support of my research.

The book was typed by Suzanne Whiter, throughout with a smile. To her my heartfelt thanks.

To my wife, Catherine, I owe an immense debt of gratitude. She has suffered happily over the years through the many referee reports of my papers. I thank her for being there with me every step of the way.

Brooklyn, NY, USA
October 2003

Viraht Sahni

References

1. M.K. Harbola, V. Sahni, Phys. Rev. Lett. **62**, 489 (1989)
2. V. Sahni, M.K. Harbola, Int. J. Quantum Chem. **24**, 569 (1990)
3. V. Sahni, M. Slamet, Phys. Rev. B **48**, 1910 (1993)
4. A. Holas, N.H. March, Phys. Rev. A **51**, 2040 (1995)

Quantal Density Functional Theory

Sahni, V.

2016, XIX, 413 p. 71 illus., 20 illus. in color., Hardcover

ISBN: 978-3-662-49840-8