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Regularity and Approximability of Electronic Wave Functions

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Preface

The electronic Schrödinger equation describes the motion of N electrons under Coulomb interaction forces in a field of clamped nuclei. Solutions of this equation depend on $3N$ variables, three spatial dimensions for each electron. Approximating the solutions is thus inordinately challenging, and it is conventionally believed that a reduction to simplified models, such as those of the Hartree-Fock method or density functional theory, is the only tenable approach. This book seeks to convince the reader that this conventional wisdom need not be ironclad: the regularity of the solutions, which increases with the number of electrons, the decay behavior of their mixed derivatives, and the antisymmetry enforced by the Pauli principle contribute properties that allow these functions to be approximated with an order of complexity which comes arbitrarily close to that for a system of one or two electrons. The present notes arose from lectures that I gave in Berlin during the academic year 2008/09 to introduce beginning graduate students of mathematics into this subject. They are kept on an intermediate level that should be accessible to an audience of this kind as well as to physicists and theoretical chemists with a corresponding mathematical training. The text requires a good knowledge of analysis to the extent taught at German universities in the first two years of study, including Lebesgue integration and some basic facts on Banach and Hilbert spaces (completion, orthogonality, projection theorem, Lax-Milgram theorem, weak convergence), but no deeper knowledge of the theory of partial differential equations, of functional analysis, or quantum theory. I thank everybody with whom I had the opportunity to discuss the topic during the past years, my coworkers both from Tübingen and Berlin, above all Jerry Gagelman, who read this text very carefully, found many inconsistencies, and to whom I owe many hints to improve my English, and particularly my colleagues Hanns Ruder, who raised my awareness of the physical background, and Reinhold Schneider, who generously shared all his knowledge and insight into quantum-chemical approximation methods. The Deutsche Forschungsgemeinschaft supported my work through several projects, inside and outside the DFG-Research Center MATHEON. I dedicate this book to my sons Klaus and Max.

Berlin, September 2009 *Harry Yserentant*

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