

Quantum Chemistry: a Challenge for Numerical Analysis

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Abstract

The basic equation of almost all quantum chemistry is the Schrödinger equation. It describes a system of electrons and nuclei that interact by Coulomb attraction and repulsion forces. The much slower motion of the nuclei is usually separated from that of the electrons. This results in the electronic Schrödinger equation, the problem to find the eigenvalues and eigenfunctions of the electronic Schrödinger operator. Solutions of this equation depend on $3N$ variables, three spatial dimensions for each of the involved N electrons. 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. We will indicate why this conventional wisdom need not to be ironclad: the unexpectedly high regularity of the solutions, which increases with the number of electrons, the decay behavior of their mixed derivatives, and their 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, depending on the spin configuration. The hope is that such properties can help to develop true discretizations of the Schrödinger equation and to incorporate recent concepts from numerical analysis into the fascinating and important field of quantum chemistry.