Multilevel Decompositions of Electronic Wavefunctions

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Abstract: With the work of Schrödinger and Heisenberg in 1926, quantum mechanics found its final form and the complete mathematical description of atoms and molecules had become possible. Dirac commented this with the words "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble." The reason is the high dimensionality of the Schrödinger equation. Its solutions depend on $3N$ variables for a system consisting of N particles, three spatial coordinates for each particle. Although very sophisticated and highly successful simplified models accessible to a numerical treatment have been developed during the last decades forming the basis of a whole branch of chemistry, from a mathematical point of view the situation has not much changed since Dirac's time. It is shown in this talk how a refined regularity theory for the electronic Schrödinger equation and modern principles of approximation theory and numerical analysis could change this situation and why the construction of true numerical methods for the Schrödinger equation comes into reach now.

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