Bernoullis Tafelrunde

Graduate Student Seminar

Monday, 9 May 2022, 12:15-13:00
Hybrid seminar
Seminar room 05.001, Spiegelgasse 5 / Zoom

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The Aufbau principle in the Theory of Operators

Abstract

A century ago the so-called Aufbau principle (German: "building up") was postulated by Niels Bohr as a model for the characterization of the electron configuration in atoms. It was based on recent experimental radiation results and on new scientific discoveries in the domain of Quantum Mechanics. The aim was to present a reasonable physical description of the ground state of an atomic system by ordering the stationary states upwards in the energy levels. Over the decades, the historic development became vague, such that in other languages one can find this principle under a different name. Today, the eigenfunctions with their eigenvalues of differential operators correspond to these stationary states at specific energy levels. Now, the Aufbau principle suggests that one should use the eigenstates that minimize a lower dimensional eigenvalue problem in order to construct the ground state solution. The result is equivalent to the minimum of the expectation value of the operator describing the higher dimensional quantum system. This interpretation provides a well defined mathematical formulation in the view of tensor products of unbounded operators acting on subdomains of Hilbert spaces. It is based on Ritz's method, which was introduced to find the solution of a variational problem by developing the solution in a linear combination of a given sequence of functions. However, without a derivation for the exact quantum chemical operator, approximations in computational methods as well as chemical experiments may display cases of violation of the principle. Modern numerical techniques in computational chemistry can benefit from this analysis in order to provide robust and physical sound models.