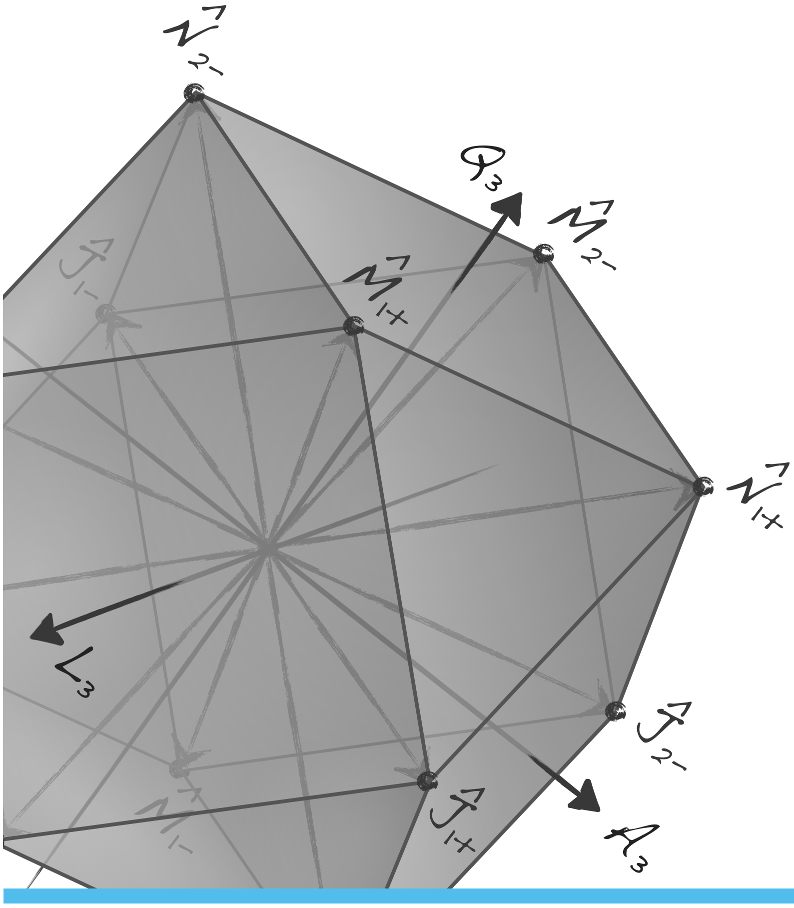
KU LEUVEN

Arenberg Doctoral School of Science, Engineering & Technology
Faculty of Science
Department of Chemistry

Symmetry and Symmetry Breaking in the Periodic Table

Towards a Group-Theoretical Classification of the Chemical Elements

Pieter THYSSEN



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Dissertation presented in partial fulfilment of the requirements for the degree of Doctor in Science

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Uitgegeven in eigen beheer door Pieter Thyssen, te Leuven.

ISBN 978-90-8649-613-6
D/2013/10.705/28

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Abstract

At the heart of chemistry lies the *periodic system* of chemical elements. Despite being the cornerstone of modern chemistry, the overall structure of the periodic system has never been fully understood from an *atomic physics* point of view. *Group-theoretical* models have been proposed instead, but they suffer from several limitations. Among others, the identification of the correct symmetry group and its decomposition into subgroups has remained a problem to this day.

In an effort to deepen our limited understanding of the periodic law, we have extended the traditional Lie algebraic framework to account for the peculiar degeneracy structure of the periodic system. Starting from the four-dimensional hidden symmetry and accidental degeneracy of the *hydrogen atom*, as first revealed by Fock in 1935, our research has mainly focussed on the way this SO(4) symmetry of the Coulomb potential gets broken in the periodic system as a consequence of the transformation of the *hydrogenic* (n, l) filling order to the *Madelung* $(n + l, n)$ order due to electronic repulsions, relativistic effects and spin-orbit couplings.

In this PhD dissertation, a new *left-step format* of the periodic table is first proposed on the basis of the Madelung rule. Following the particle physics tradition, the chemical elements are then considered as various *states* of some '*atomic matter*', which is described by a non-compact spectrum-generating dynamical Lie group. The chemical elements are shown to form a basis for a single infinite-dimensional degeneracy space of the SO(4,2) $\otimes$ SU(2) group. An explanation for the *period doubling* is then proposed in terms of a particular symmetry breaking of the SO(4,2) group to the anti de Sitter SO(3,2) group. The Madelung rule is rationalized on the basis of *nonlinear* Lie algebras which reflect the screening of the Coulomb hole. This opens new perspectives for a symmetry-based understanding of how the periodic law emerges from its quantum mechanical foundations, and holds the future promise of complementing our current *phenomenological* approach by a direct *atomic physics* approach.