Towards a Relativistically Covariant Many-Body Perturbation Theory

- With Numerical Implementation to Helium-Like Ions

Daniel Hedendahl

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Fakultetsopponent:	Professor Stephan Fritzsche Department of Physical Sciences, University of Oulu Helmholtz Centre for Heavy Ion Research, GSI Darmstadt
Examinator:	Professor Ann-Marie Pendrill Institutionen för fysik, Göteborgs universitet
Huvudhandledare:	Docent Sten Salomonson Institutionen för fysik, Göteborgs universitet

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GÖTEBORGS UNIVERSITET

Institutionen för fysik
Göteborgs universitet
412 96 Göteborg
Sweden

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Daniel Hedendahl
Department of Physics
University of Gothenburg
412 96 Gothenburg, Sweden

Abstract

The experimental results for simple atomic systems have become more and more accurate and in order to keep up with the experimental achievements the theoretical procedures have to be refined. Recent accurate experimental results obtained for helium-like ions in the low- and moderate-Z regions proclaim the importance of theoretical calculations that combines relativistic, QED and electron correlation effects. On the basis of these premises the relativistically covariant many-body perturbation procedure is developed and it is this development that is introduced in this thesis. The new theoretical procedure treats relativistic, QED and electron correlation effects on the same footing.

The numerical implementation leads to a systematic procedure similar to the atomic coupled-cluster approach, where the energy contribution of QED effects are evaluated with correlated relativistic wave functions. The effects of QED are also included in the resulting numerical wave functions of the procedure, which can be reintroduced with an approach of iteration for calculations of new higher-order effects.

The first numerical implementation of the procedure to the groundstate for a number of helium-like ions in the range $Z = 6 - 50$ of the nuclear charge, indicates the importance of combined effects of QED and correlation in the low- and moderate-Z regions. The results show also that the effect of electron correlation on first-order QED-effects for He-like ions in the low and moderate-Z regions dominates over second-order QED-effects.

Keywords: many-body perturbation theory, bound state QED, helium-like ions, Green's operator, covariant evolution operator, combined effects of QED and correlation, atomic structure calculations