Molecular Quantum Electrodynamics:
theoretical and computational developments
Semester report: 1. semester

Particle and Nuclear Physics program

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1 Introduction

Atoms and molecules are bound systems in which the dominant interaction is the electromagnetic force. A correct relativistic description requires a field-theoretical treatment of this interaction.

In atomic physics, quantum electrodynamical (QED) corrections are calculated within the bound-state QED framework, an effective theory based on the Dirac equation in the external field of the nucleus. These corrections are crucial in strong fields. Furthermore, several theories beyond the Standard Model are particularly sensitive to strong electric and magnetic fields. Therefore, a better understanding of the spectra of heavy elements can lead to new discoveries in fundamental physics [1]. The aim of my research is to develop theoretical and computational frameworks to examine corrections in strong Coulomb fields.

2 Research

In my research, my main focus lies on the leading-order vacuum polarization correction in bound systems. In bound-state QED, the leading-order vacuum polarization

correction is incorporated into the following vector potential::

$$A^a_{\mathrm{VP},\nu}(\boldsymbol{y}) = -\frac{e}{4\pi}\int d^3x \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|}\mathrm{Tr}[\gamma_\nu G_a(\boldsymbol{x},\boldsymbol{x})]\,.$$

This potential has several desirable properties: only the scalar part of the potential is non-zero, which describes an instantaneous interaction. On the other hand, the potential is divergent. One possible solution to this problem is to replace the bound-electron propagator with its Dyson series,

$$G_a(x_1,x_1') = G_a^{(0)}(x_1,x_1') - \mathrm{i}\int d^4y_1\, G_a^{(0)}(x_1,y_1)\gamma_0 V_a(y_1) G_a(y_1,x_1')\,.$$

This procedure generates a power series for the bound vacuum polarization potential,

$$V^a_{\mathrm{VP}} = \sum_0^\infty V^{a,(n)}_{\mathrm{VP}}\,.$$

It can be shown that only the first-order term is divergent, but this term can be renormalized analytically. The renormalized correction is the well-known Uehling potential,

$$V^a_{\mathrm{U}}(r) = -\frac{2\alpha}{3\pi}\frac{(Z\alpha)}{r}\int_1^\infty dx\, \mathrm{e}^{-2m_a x r}\frac{2x^2+1}{2x^4}\sqrt{x^2-1}\,.$$

During this semester, I implemented the Uehling potential for atomic systems. In the calculations, the Uehling potential is inserted into the Dirac equation, which provides a non-perturbative treatment of the vacuum polarization correction of order $\alpha(\alpha Z)$. I performed calculations for hydrogen-like and helium-like systems and found good agreement with NRQED results.

At the end of the semester, I began working out the details of molecular calculations. In the coming months, I plan to implement the molecular calculation and write an article on the calculation of the Uehling correction in atomic and molecular systems.

3 Conferences and talks

- I attended the Molecular Response Properties Summer School (MRPSS) in Stockholm, Sweden. I also presented a poster during the summer school.
- I gave a talk about my research in Lindköping, Sweden.
- I gave a popular science talk about field theories at ELTE BTK.

4 Studies

This semester I attended three courses:

- Astroparticle physics (FIZ/2/132)
- Integrable field theories (FIZ/2/084E)
- Algebraic quantum field theory 1. (FIZ/2/020E:2)

5 Teaching

This semester I was teaching two courses:

- Introduction to computational tools (2 hours a week)
- Physics of Atoms, Nuclei, and Elementary Particles, practice (1 hour a week)

I also wrote a lecture note to the practice of the Physics of Atoms, Nuclei, and Elementary Particles.

References

[1] Ch. Orzel. *New Physics Searches Using Precision Spectroscopy*, page 337–375. Elsevier, 2018.