

Although effects between external magnetic field and nuclei are extremely subtle, they can give a lot of information about atoms and molecules. Nuclear Magnetic Resonance spectroscopy (NMR), which measure those interactions has a wide application - from determination of the exact molecule structure, up to medical imaging.

Similar to other experimental methods, development of the NMR spectroscopy is limited not only by apparatus, but also by precision of the reference values used in measurement. The universal standard in NMR spectroscopy is shielding of helium-3, which can be determined only theoretically. Interestingly, to obtain accurate result which will meet the needs of modern technology, using quantum mechanics formed by Schrödinger is no longer enough. Although it predicts properties of atoms quite accurately, it is not efficient for NMR technique. Only through application of quantum electrodynamics - the most accurate theory known - it is possible to obtain fully satisfying result. Consideration of effects induced by presence of two electrons in helium atom presents particular challenge. Development of formalism which would consider electronic correlation is non-trivial task as similar studies were performed only for hydrogen-like systems.

The final result of this project will be an ultraprecise calculation of the shielding constant for the helium-3. Possibility of using the most fundamental theoretical methods and calculations of high precision will enable to obtain result, which will set new standards of accuracy and will be a reference to more complex systems.