1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Highly accurate quantum mechanical modeling of Rydberg atoms confined in magnetic or optical traps. Application in designing qubit memory arrays for quantum computers

1.1. **Project goals** These are the main goals of the project: (1) Development of quantum mechanical methods for modeling individual atom trapped by optical or magentic fields using an approach where the motion of nuclei are treated on equal footing with the motion of the electrons; (2) Development of a quantum-mechanical approach to model entanglement of Rydberg states of separated atom in traps for its use in constructing qubit memory arrays for quantum computing.

1.2. **Outline** An interesting problem to study is bound states of atoms and molecules spatially confined by optical and magnetic traps, or confined to cages formed by molecular networks. The non-Born Oppenheimer approach and the explicitly correlated Gaussians with shifted centers are very well suited to calculate such states, which can be either internal states, or translational/rotational states, or have characteristics of both types of states. The study of confined molecules is related, for example, to storing hydrogen gas in molecular cages as fuel. The study of confined atoms is related, for example, to use of single Rydberg atoms as so-called qubits in quantum computers. Another example is the behavior of small molecular systems in interstellar space trapped by quickly rotating, very strong magnetic fields. Molecular phenomena related to the interaction with very strong magnetic fields cannot be studied in the laboratory because such magnetic-field strengths are not attainable on earth. The project involves development of algorithms for performing highly accurate quantum mechanical calculations of atoms excited to Rydberg states and interacting with magnetric and optical fields. The algorithms will be implemented on multiprocessor computer systems using parallel protocols. The work will involve writing efficient computer codes and executing them using parallel processing. It will also involve running the codes and modeling possible use of matrices of trapped individual atoms as qubit memory units in quantum computers. The phenomenon of quantum entanglement of atomic Rydberg states will be employed in the modelling.

1.3. Work plan It is expected that project will last up to four years. In the first year the work will be devoted to creating the model of trapped individual atoms trapped by an magnetic or optical field and their Rydberg states forming coherent superposition of states. In the second year, the algorthms will be implemented and computer codes will be written and tested. In last two years three and four the software will be used to model qubit trapped Rydberg-atom arrays for their possible use as memory units in quantum computers.

1.4. Literature

2. L. Adamowicz, M. Stanke, E. Tellgren, and T. Helgaker, Explicitly-correlated non-Born-Oppenheimer calculations of the HD molecule in a strong magnetic field, Chem.Phys.Lett. **682**, 87 (2017).
3. L. Adamowicz, M. Stanke, E. Tellgren, and T. Helgaker, A computational quantum-mechanical model of a molecular magnetic trap, J. Chem. Phys. **149**, 244112 (2018).
4. A.Browaeys, T. Lahaye, Many-body physics with individually controlled Rydberg atoms,Nature Physics, **16**, 132-142 (2020)
5. A.Mitra, M.J.Martin, G.W.Biedermann,A.M.Marino,P.M. Poggi,I.H. Deutsch, Robust Molmer-Sorensen gate for neutral atoms using rapid adiabatic Rydberg dressing, Phys.Rev. A, **101**, 030301 (2020)

1.5 Required initial knowledge and skills of the PhD candidate the required skill:
knowledge of quantum mechanics, the basics of programming, commitment to work, skills in writing computer codes using parallel protocols, large-scale application calculations on multiprocessor computers are welcome.

1.6 Expected development of the PhD candidate's knowledge and skills :
Development of knowledge of application of quantum mechanics to calculate spectra of atoms and molecules at high level of accuracy. Development of the ability to carry out derivations of complex algorithms in the area of atomic and molecular quantum mechanics. Development of skills in writing complex computer programs using parallel protocols and in implementing these programs on large parallel computer systems.