Popular Summary

Next year the International System of Units (SI), forming a basis for highly accurate, traceable measurements in science and technology, will undergo a fundamental change. It will no longer be based on artifacts like the platinum-iridium cylinder kept in Saint-Cloud in France and serving as the prototype of the kilogram, but will employ well defined atomic properties and fundamental laws of physics for the definition of its basic units. Specifically, the energy of one joule and the temperature of one kelvin will be defined as exactly specified multiples of the energy of a single photon emitted during the hyperfine transition in the cesium atom, the same transition that has been used since 1967 for the definition of the second and meter. These new definitions will enable more precise measurements of temperature and pressure, which is important in many areas of human activity from vacuum manufacturing of semiconductor chips to aviation and marine navigation.

The objective of the proposed research is to develop theory and computer programs enabling accurate prediction of atomic properties that are critical for the development of better, atomic standards of pressure and temperature. Specifically, these critical properties are the electric and magnetic properties of noble gas atoms and the parameters characterizing interactions of these atoms in the vacuum and in laser fields. The quantum mechanics in the Schrödinger formulation predicts atomic properties quite accurately but, since it violates the principles of the Einstein theory of relativity, its accuracy is not good enough for the purposes of modern metrology. Fortunately, physicists discovered how to reconcile quantum postulates with Einstein's relativity and the resulting theory of quantum electrodynamics is presently the most precise theory in science − for one- or two-electron atoms its predictions agree with experiment to one part per billion or better. This theory will be used by the researchers of this project to predict electric properties of noble gas atoms with precision sufficient for the purpose of temperature and pressure metrology. The proposed research will require quantum and relativistic modeling of a system containing up to three dozen of electrons - the task very challenging even at the level of the standard non-relativistic quantum theory of Schrödinger.

The final result of the project will be algorithms and general computer programs for accurate prediction of atomic properties as well as an application of these programs for accurate determination of a few specific atomic parameters relevant for the development of new metrology standards. One of such standards − the optical standard of pressure is now under development at the National Institute of Standards and Technology (NIST) in Maryland, USA. The parameters needed for a successful construction of this standard describe the response of individual atoms (and atomic pairs) to external electric and magnetic fields. A small, desktop optical instrument, designed by NIST's researchers to determine pressure from ultra-precise measurements of the refractive index of noble gases, will replace the current apparatus − a three-meter tall column containing a quarter of a tonne of neurotoxic, environmentally hazardous mercury. The new mercury-free optical pressure standard, resulting from the combination of advances in laser interferometry and fundamental quantum calculations, is expected to benefit many branches of science, and, after further miniaturization, may become a commercial device used across industry, academia, and in everyday life.