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Editorial

Some Current Trends in Atomic Theory

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Atomic theory continues to develop even after a century of rapid progress. Several times during this period, atomic physics were at the frontier of the physical studies. The most recent growth of the interest to atomic physics was caused by the dramatic increase in the accuracy of atomic experiments after the development of cooling and trapping techniques. At present, these techniques are beginning to be applied to molecules and highly charged ions promising rapid increase in accuracy of the experiments with these species in the near future.

Because of these tendencies, the atomic systems, including atoms, ions, and molecules, continue to serve as precision instruments to study fundamental physics and to test new theoretical models. For example, atomic experiments are used to search for: violation of the fundamental symmetries, including parity, time-reversal, and Lorentz-invariance violation; possible variation of the fundamental constants from the cosmological time-scale to the oscillations at radio frequencies; exotic interactions mediated by light bosonic fields, which are predicted by some models of the dark matter and dark energy. High precision atomic data are required for development of atomic clocks, planning experiments with ultracold atoms, astrophysics, and plasma physics. In all these studies, we use not only high precision experimental methods of atomic physics, but also comprehensive calculations of various properties of atoms and molecules. This Special Issue is devoted to the new theoretical and computational methods in atomic physics, which bridge the gap between the atomic observables and the parameters of the fundamental theories.

The present level of accuracy required accounts for quantum electrodynamics (QED) effects not only for the simplest one-, or two-electron atoms, but also for many-electron atoms and molecules. Three papers of this Special Issue are devoted to the QED calculations of the bound many-electron systems [1–3]. Yerokhin et al. [1] describe high order QED calculation of He with the help of the two-electron exponential basis functions. Using such basis functions allows them to account for electronic correlations very effectively. After that, perturbation theory is used to calculate QED corrections. Comparison of the calculated transition energies with the high precision experiments reveal some small, but systematic deviations. The authors conclude that more efforts are needed from both sides to resolve these discrepancies.

Soguel et al. [2] use the redefined vacuum approach for the bound-state QED perturbation theory of many-electron systems. This approach drastically reduces the complexity of the many-electron QED expressions keeping only valence electrons, or vacancies under consideration. Applying this method to the particular case of an atom with one hole in the closed shells, they calculate all first- and second-order many-electron contributions. The authors conclude that redefined vacuum approach provides a straightforward derivation for any electronic configuration within rigorous QED framework.

For atoms with the nuclear charge $Z \gg 1$ the theoretical treatment of QED effects must be performed without expansion in the parameter $Z\alpha$, where α is the fine-structure constant. Such calculations require numerous summations over the Dirac spectrum in the presence of the nuclear potential. Respective sums can be evaluated with the help of the Dirac Green function (DGF). Yerokhin and Maiorova [3] contributed a short review

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about using DGF for the QED calculations of complex atoms. Most widely used numerical representations of DGF are applicable for a broad range of spherically symmetric potentials. This allows them to account for finite nuclear size effects and the screening caused by the presence of other electrons in the atom. The dominant uncertainty of this method usually comes from the truncation of the partial-wave expansion. The authors conclude that in calculations using DGF, it is important to find universal approach to improve the convergence of the partial-wave expansion.

For the atoms with several open shells, an accurate treatment of the correlation effects becomes extremely difficult and computationally expensive. At the same time, such atoms may have very high sensitivity to small perturbations and, therefore, to the new physics. Such atoms may also have convenient transitions for optical clocks and are important for astrophysics and plasma physics. That is why it is very important to develop new effective computational methods for such systems. Contributions Cheung et al. [4] and Fritzsche et al. [5] describe two modern packages for atomic calculations. The first package implements configuration interaction (CI) plus many-body perturbation theory (MBPT) calculations of the spectra, transition amplitudes, and other properties of the complex many-electron atoms. The dimension of the CI space grows exponentially with the number of valence electrons. Therefore, for the atoms with more than four valence electrons the size of the CI space is extremely large and parallel computations are absolutely necessary. The package described by Cheung et al. [4] demonstrates near-perfect linear scalability and efficiency with the number of processors used for the calculation, giving hope that soon most open-shell systems will be treated with sufficiently good accuracy.

Atomic cascades are ubiquitous in nature. They happen, for example, after the excitation of the one of the inner shell electrons of the many-electron atom and they have been explored within very different scenarios, from precision measurements to the modeling of the radiation damage in biological substance. Fritzsche et al. [5] suggest a classification of atomic cascades and demonstrate how they can be modeled with the help of the Jena Atomic Calculator (JAC) package. As an example, the authors compute the stepwise decay cascade of atomic magnesium, following ionization of a 1s electron. The authors argue that JAC package can be used for a broad variety of the cascade processes in atoms.

Polarizabilities of atoms are needed in many areas of physics and chemistry. For example, dynamic polarizability determine the shift of the atomic clock transition in the external field of the optical lattice. At the same time calculation of polarizabilities requires summation over atomic spectrum and is very difficult for the many-electron atoms. Instead of the explicit summation over the intermediate states one can solve inhomogeneous equation in the CI space. This method significantly simplifies calculations, but is still computationally very expensive for atoms with many electrons in the open shells. Further simplification can be achieved if CI method is combined with the perturbation theory. Dzuba [6] describes the extension of the method of inhomogeneous equation for the combination of the CI with the perturbation theory. The author demonstrated the effectiveness of this method by calculating polarizabilities of the ground and excited states of such complex atoms as Er, Tm, and Yb.

An accuracy of the molecular experiments is growing very fast and has reached the level, which was recently possible only for atoms. At the same time, molecules are much more sensitive, for example, to the violation of the inversion symmetry P and time-reversal invariance T. That requires accurate calculations of the respective effects for a variety of molecules including heavy ones. Many such calculations use relativistic coupled cluster (CC) method, or its linearized version. Numerous calculations of the effective electric field on the unpaired electron were done within linearized CC method. This effective field determines the P,T-odd effect induced by the electric dipole moment of the electron. Prasannaa et al. [7] calculated non-linear corrections to the effective electric field for several heavy diatomic molecules and found them to be between 1% and 2%. This means that linearized CC method appears to be sufficiently accurate for the effective field in the

considered molecules. However, the authors point out that there are large cancellations between different non-linear terms and therefore these terms should be included for the reliable predictions.

Parity non-conservation (PNC) effects were accurately measured for several atoms. However, nuclear-spin-dependent (NSD) PNC effects have not been reliably observed for atomic systems. In heavy atoms and molecules these effects are predominantly induced by the anapole moment of the nuclei. This moment appears because of the PNC interactions inside the nucleus. Only in atomic and molecular hydrogen the NSD PNC effect is induced purely by the electron-proton weak neutral current. Therefore, only experiments with hydrogen may allow to measure respective coupling constant. Chubukov et al. [8] report results of the calculation of the NSD PNC amplitude for the M1 vibrational transition in the ortho-hydrogen molecule and estimate PNC optical rotation for the high-finesse optical cavity experiment. The angle of rotation of the plane of polarization of light appears to be about 3×10^{-13} rad, which is close to the smallest angle measured so far in the optical cavity experiment.

We see that the papers published in this Special Issue address different hot topics of the modern atomic theory from studying violations of the fundamental symmetries to the predicting properties of the complex atoms with many valence electrons. Several papers discuss different aspects of the application of the QED methods for the high precision atomic calculations. Several other papers are devoted to the development of the methods to effectively account for the electronic correlations in many-electron atoms and treating very complex cascade processes. Two papers consider effects of the violation of the parity and time-reversal invariance in diatomic molecules and suggest new experiments to search for these effects. All these directions of atomic theory are rapidly developing and attract the attention of many researchers. Because of that, we hope that this Special Issue will be in demand by specialists and will stimulate new research in the areas outlined here.

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