PARITY NONCONSERVATION IN ATOMS AND MOLECULES

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Theory of the parity nonconservation (PNC) and the break of time-reversal invariance in atoms and molecuies is one of the traditional fields of the research in PNPI. Lately, the accent was made on the calculation of these effects for the atoms and molecules where experiments are now underway, in particular, diatomic radical YbF [1] and atoms Dy [2], Bi [3] and Yb [4].

The main interest in YbF molecule is caused by the possibility to improve existing limit on the electric dipole moment of the electron, which follows from the experiment with atomic Tl. Calculation [1] is based on the semiempirical model of the diatomic radical in $^2\Sigma_{1/2}$ state which provides the 20% accuracy for the PNC effects (for the general discussion of the PNC in diatomics see review [5]).

Atomic calculations [2-4] were made using the *ab initio* relativistic configuration interaction (CI) method. Rare-earth atoms Dy and Yb are interesting because of the large enhancement of the PNC effects and because of the large number of stable even isotopes. The latter allows to stydy the dependance of the PNC effects on the number of neutrons in the nucleus. Unfortunately, electronic wave function for Dy is very complicated and the accyracy of calculation is not high [2]. Electronic structure of Bi and Yb is simplier, but still electronic correlations (including core-valence correlations) are very important [3,4]. PNC experiment on bismuth [6] reached the accuracy which allows to look for the nuclear spin-dependent PNC effects. In [3] the first *ab initio* calculation of these effects has been made.

Further improvement of the accuracy of atomic calculations can be achieved by the combination of the CI for the valence electrons with the many-body perturbation theory for the core-valence correlations. Our first calculations of the ionization potentials and low-lying energy levels of Tl and Ca show that the accuracy of this combined method is about an order of magnitude higher than conventional CI.

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