Breit interaction in heavy atoms.

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It is well known that in high accuracy atomic calculations one may need to go beyond the Coulomb approximation for the two-electron interaction. The usual next step is to include the Breit interaction. A number of commonly used atomic packages, such as GRASP package [1], allows to do this rutinely. However, in many precision calculations one needs to account for different corrections, which are not included in standard packages. Thus, it may be important to analyze the role of the Breit interaction on different stages of atomic calculations. Below we present several simple observations which may help to include Breit interaction in atomic calculations in an optimal way.

Let us note, that we restrict this discussion in two ways. First, we discuss only the so-called Gaunt term of the Breit operator. This term is known to dominate in atomic calculations and it is much simpler than the whole Breit operator (see [2] for details). Second, we are interested in the calculations of the low-energy properties of heavy atoms. In such calculations all electrons are usually divided into two parts: the core electrons and the valence electrones. Correspondingly, the interaction between electrons is reduced to the interaction between the valence electrons and the interaction of the valence electrons with the atomic core. The latter is described by the Dirac-Fock potential which includes direct and exchange terms. In this case the following simple observations may be made.

- Breit correction to the interaction between the valence electrons is of the order of α^2 (α is the fine structure constant) which is usually below the accuracy of modern calculations.

- Breit correction to the direct term of the Dirac-Fock potential turns to zero if the core includes only closed shells. Indeed, the vertex of the Breit interaction includes Dirac matrix $\vec{\alpha}$, which is averaged to zero when summation over the closed shell is done.

- Breit correction to the exchange interaction of the valence electron with the core does not turn to zero and is of the order of R^2, where R is the overlap integral between the upper component of a valence orbital and the lower component of a core orbital. The largest integrals R correspond to the innermost core orbitals, where small components are of the order of αZ.

- The exchange interaction between valence electrons and the innermost core electrons is significantly screened if the core relaxation is allowed. Therefore, it is very important that Breit correction to the core potential is calculated self-consistently. In some cases

the core relaxation can reduce the final Breit correction to the valence energies by an order of magnitude.

If the many-body perturbation theory in residual Coulomb interaction is used to account for some types of correlations, one may need to include Breit corrections to corresponding diagrams. Generally speaking, there are two types of corrections: "direct" and "indirect" ones. The former correspond to the substitution of the residual Coulomb interaction by the Breit interaction and the latter correspond to the use of the orbitals which are obtained by solving Dirac-Fock equations with Breit potential. The "direct" corrections are suppressed because the largest Breit radial integrals correspond to the virtual excitations from innermost core shells and these excitations correspond to huge energy denominators. Therefore, one can neglect them without significant loss of accuracy. This essentially simplifies calculations.

At the conference we will give some numerical results for Breit corrections to differenct observables in Cs and Tl.

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