Relativistic adiabatic time-dependent density functional theory using hybrid functionals and noncollinear spin magnetization

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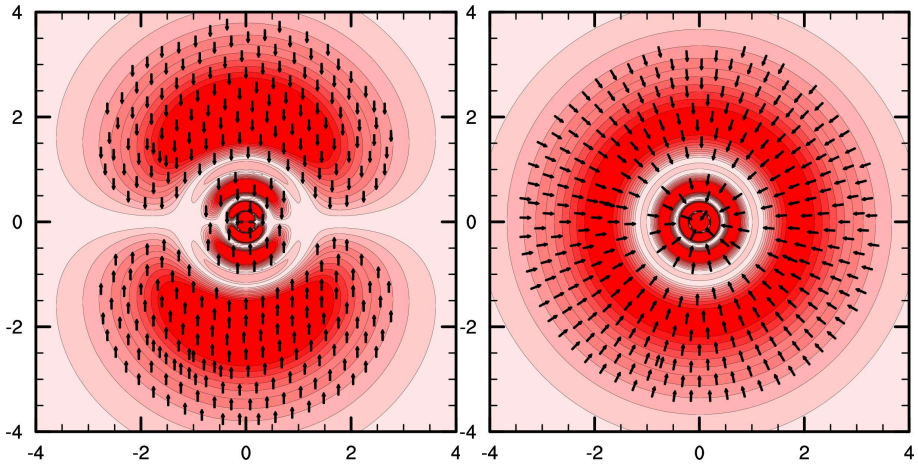

Induced spin magnetization for the first $6s^2 \rightarrow 6s6p$ excitation in Hg (non-relativistically $^3P_0$), with (right) and without (left) spin-orbit coupling.

In my talk I report an implementation of adiabatic time-dependent density functional theory based on the 4-component relativistic Dirac-Coulomb Hamiltonian and a closed-shell reference. The implementation includes noncollinear spin magnetization and full derivatives of functionals, including hybrid generalized gradient approximation (GGA) functionals. We avoid reducing the generalized eigenvalue problem to half the dimension involving the square of excitation energies since this may introduce spurious roots and also squares the matrix condition number. Rather we impose structure in terms of hermiticity and time reversal symmetry on trial vectors to obtain even better reductions in terms of memory and run time, and without invoking approximations. Further reductions are obtained by exploiting point group symmetries for D_{2h} and subgroups in a symmetry scheme where symmetry reductions translate into reduction of algebra from quaternion to complex or real. For hybrid GGAs with noncollinear spin magnetization we derive a new computationally advantageous equation for the full second variational derivatives of such exchange-correlation functionals. Selected applications will be presented.