GEN1INT: An object-oriented library to evaluate one-electron integrals and their derivatives

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We have recently proposed a procedure for evaluating one-electron integrals and their geometric derivatives by using a generalized one-electron operator that is the product of four factors: (1) a scalar $(X_\kappa - X_\lambda)^{K_X}(Y_\kappa - Y_\lambda)^{K_Y}(Z_\kappa - Z_\lambda)^{K_Z}$ depending on the relative displacement of the two basis function centers $\boldsymbol{R}_\kappa$ and $\boldsymbol{R}_\lambda$, typically arising from the differentiation of London atomic-orbitals (LAO) with respect to the external magnetic field; (2) a multipole-moment operator $(x - M_x)^{m_x}(y - M_y)^{m_y}(z - M_z)^{m_z}$ around the origin $\boldsymbol{M}$, arising from the differentiation with respect to the external electric field; (3) an arbitrary central-potential operator $f(|\boldsymbol{r} - \boldsymbol{C}|)$ around center $\boldsymbol{C}$, and (4) an electronic differential operator $(\partial/\partial x)^{n_x}(\partial/\partial y)^{n_y}(\partial/\partial z)^{n_z}$ [1]. This procedure has been extended in a more recent work [2] by including molecular magnetic properties, leading-order relativistic corrections from the one-electron part of Breit–Pauli Hamiltonian, effective core potential, and model core potential (Version 1). The evaluation of these integrals is performed by using LAOs to ensure the origin independence. The derivatives of the integrals with respect to the external electric and magnetic fileds, nuclear point magnetic moment, and geometry perturbation have been thoroughly considered, and implemented in an open-ended integral library GEN1INT.

In this presentation, I would like to briefly describe the theoretical background of this integral library GEN1INT, and then focus on its structures, functionalities and limitations, usage and performance. The purpose of this presentation is to make this library be known and useful in the quantum chemistry community.

[1] Bin Gao, Andreas J. Thorvaldsen and Kenneth Ruud, *Int. J. Quantum Chem.*, in press, DOI: 10.1002/qua.22886 (2010)

[2] Bin Gao, Kenneth Ruud and Trygve Helgaker, in preparation (2010)