Efficient computation of Coulomb integrals and their applications to collision problems in quantum mechanics

Coulomb (or two-electron) integrals are an essential quantity needed by many computational approaches for studying multi-electron quantum mechanical systems such as molecules. These are 6-dimensional multi-center integrals describing the electron-electron interaction. In most applications the functions being integrated are Gaussians which leads to well-known analytic formulae for the Coulomb integrals. Recently, computer codes specialized to problems of collisions of electrons with molecules have switched to using numerical functions (B-splines) for the description of the unbound particle. While this opens a wide range of new problems that can be investigated it also leads to the necessity of computing a large number (billions) of mixed-basis Coulomb integrals involving Gaussians and B-splines. In our computer codes we have implemented a method based on the Legendre expansion for computation of the Coulomb integrals which has been very successful but has several limitations, especially in case of the mixed exchange integrals.

In this work we will focus on development of an alternative numerical method for computation of the Coulomb integrals based on solving the Poisson equation using the R-matrix approach known from quantum mechanics. This approach should lift the limitations of the Legendre approach to the integral computation and lead to a more efficient code which will open the way to new applications.

This project is flexible and can be carried out either as a bachelor or a diploma thesis.

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References:

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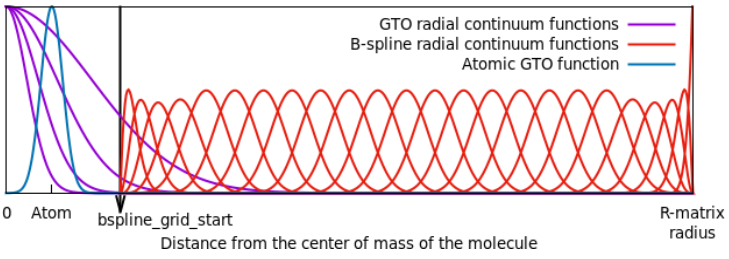

$$(ij|kl) = \int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2 \frac{\phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_1)\phi_k(\mathbf{r}_2)\phi_l(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$