

Scientific Report: Automatic Analytical Computation of Exact Kinetic Energy Operators in the Context of Curvilinear Coordinates

The research stay with the group of Dr. David Lauvergnat proved very fruitful to my understanding of curvilinear coordinates in general and the specific class of polyspherical coordinates in particular. I was able to acquire the necessary mathematical understanding of kinetic energy operators in a curvilinear context to provide foundation for the programming aspects of this projects. This understanding was obtained through both discussions and formally solving the associated equations together with Dr. David Lauvergnat.

There exists both numerical and analytical approaches to handling the kinetic energy operators but we chose to focus our attention on the analytical approach by means of the TANA program, which is developed in the group of Dr. David Lauvergnat. The exploration of the TANA program together with the advices given by Dr. David Lauvergnat provided an excellent basis for implementing an interface between the TANA program and the MIDASCPP suite of the Ove Christiansen group.

Progress proved to be faster than initially anticipated and I was able to implement several core features in this interface between TANA and MIDASCPP during the research stay. Additional work still remains but I am very optimistic about being able to perform calculations within a reasonable time frame.