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Work plan:
Automatic Analytical Computation of Exact Kinetic Energy Operators in the Context of Curvilinear Coordinates

The central topic of my PhD project is efficient construction of the Hamilton operator for nuclear motion, which naturally leads to the question of which coordinate representation should be used. I have previously been working with various rectilinear coordinates but these have natural restrictions due to their nature and a much more adequate representation can be obtained by switching to curvilinear coordinates, i.e. distances and angles. This representation unfortunately means that the kinetic energy operators becomes quite complex, which is in stark contrast to the use of e.g. rectilinear Cartesian coordinates.

Dr. David Lauvergnat is an expect in handling these complex kinetic energy operator expressions in an automated fashion and the aim is to obtain an understanding of how his group undertake this ordeal. There exists both numerical and analytical approaches to overcome the problems with the kinetic energy operators but this project will mainly be focused on the analytical approach. To that end, becoming familiar with the locally developed TANA program, which handles the computational aspects of determining kinetic energy operators is a key component.

This collaboration is expected but not necessarily restricted to cover the following aspects:

- An in-depth understanding of the mathematical foundation of kinetic energy operators in a curvilinear coordinate context.
- The analytic approach to dealing with the kinetic energy operators within a curvilinear coordinate context uses a parametrization of the molecular system in polyspherical coordinates. Naturally, an understanding of this particular set of coordinates is a key point.
- Acquire detailed knowledge of the TANA program.
- Interface the TANA program with the MidasCpp suite of the Ove Christiansen group in order to take advantage of the unique features found in both programs. This might might including addition programming work on integral evaluation.
- Investigate the behaviour of potential energy surface and vibrational coupled-cluster algorithms native to MidasCpp with a curvilinear coordinate representation for various small to medium sized molecules.