IWR-Colloquium WS 2014/2015

November 19, 2014
17:15h
IWR, Im Neuenheimer Feld 368, 69120 Heidelberg, Room 432

Speaker:
Dr. James Emil Avery, University of Copenhagen

Title:
"Hyperspherical Harmonics and Molecular Integrals"

Abstract:

In this talk, I will show how the theory of hyperspherical harmonics can be used to solve multi-centre integrals that arise in molecular calculations.

I will present a general and efficient method for exact angular integration for any dimensionality, and show how it can be used together with V.A. Fock's transformation of momentum space to the unit hypersphere to find simple closed form solutions to molecular integrals where available, and efficient approximations where closed form solutions do not exist.

A prototype software library that implements the discussed methods will be reviewed.

Website:
www.iwr.uni-heidelberg.de/iwr-colloquium