UNIVERSITÉ CÔTE D'AZUR

GRADUATE SCHOOL
FORMAL, PHYSICAL AND ENGINEERING SCIENCES

1) Field of study : Scientific computing, quatum chemistry

2) Internship topic : Representation of distorted hydrogen orbitals using Gaussians functions

3) Description :

We recently proposed to use deformed hydrogen orbitals (OHDs) in order to solve the molecular Schrödinger equation, by the EN-MFCI method (Electron- Nucleus Mean Field Configuration Interaction), see [1, 2, 3]. OHDs are functions of $\mathbb{R}^3$ to $\mathbb{R}$ from which an asymptotic expansion can be obtained as a function of a parameter measuring the deviation from sphericity: they tend towards the usual hydrogen orbitals (the the spherically symmetric orbitals of chemists) when this parameter tends towards zero. However, to use these OHDs functions effectively in quantum chemistry computations, it is appropriate to substitute a representation in the form of a linear combination of Gaussian functions, possibly added with a polynomial prefactor. The internship will consist to establish such a representa- tion for lower energy OHDs. This could be done by quadrature using a software of formal computing. We will study the convergence according to the number of involved Gaussian functions and depending on the order of asymptotics expansion of OHDs. Gaussian OHDs will then be introduced and used in the Chinese code of quantum chemistry BDF (http://182.92.69.169:7226/Introduction) and this work can be continued in thesis.

References [1] P. Cassam-Chena, G. Lebeau, Smeared Coulomb potential or- bitals: I-asymptotic expansion sion, J. Math. Chem. 59, 985 (2021).
[2] P. Cassam-Chena, B. Suo, W. Liu, Decoupling electrons and nuclei without the Born- Oppenheimer approximation: The Electron-Nuclei Mean-Field Config- uration Interaction Method, Phys. Rev. A92, 012502 (2015).
[3] P. Cassam-Chena, B. Suo, W. Liu, A quantum chemical definition of electron- nucleus correlation, Theor. Chem. Acta. 136, 52 (2017).

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4) Internship level :	Master 2
5) Requirements :	Basic background in scientific computing
6) Duration :	3 to 6 months
7) Period :	February to July 2024
8) Laboratory :	LJAD
9) Contact :	Patrick Cassam-Chenaï, Patrick.CASSAM-CHENAI@univ-cotedazur.fr, chargé de recherche, Laboratoire Jean Alexandre Dieudonne (LJAD/CNRS UMR7351) – Université Côte d'Azur, 28, avenue Valrose, 06108 Nice Cedex

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