Training Stage Proposal MSIAM

Wavelets on the Interval for Schroedinger Equation

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Possiblity of a PhD thesis : Yes

Introduction and context

The Kohn-Sham (KS) formalism of the Density Functional Theory (DFT) approach [**?**] is the most widely used first-principles method for investigating properties of atomistic systems. The computational machinery of DFT calculations has been widely developed in the last decade, giving rise to a plethora of DFT codes. The usage of DFT calculation has thus become more and more common, and its domain of application includes solid state physics, chemistry, materials science, biology and geology. An efficient electronic structure program will make the analysis of more complex systems and environments possible, thus opening a path towards new discoveries.

In this project, we will explore the potential advantages of a newly conceived formalism for DFT, implemented in the BigDFT [**?**] electronic structure code. This code uses Daubechies wavelets to express the solution of the Schroedinger Equation.

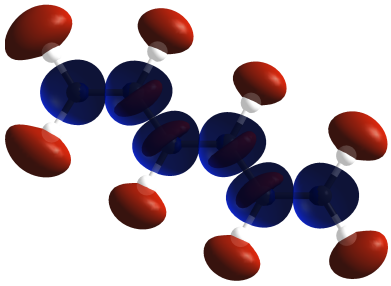
The training will be based on the usage of the wavelet-on-the-Interval family [**?**] to perform accurate and efficient solution of the Schroedinger equation without finite-size effect. Ideally, the trainee should have interest in the subject of Applied Mathematics. The training will be mainly focused on the resolution of the one-dimensional Schroedinger equation in the basis of wavelet-on-the-interval. The outcome of the training might lead to interesting scientific publication. Depending on his/her interests/skills, the candidate will then have the possibility to continue to work in the electronic structure calculation community in a PhD thesis, which will be focused on the enhanced potentialities of BigDFT code.

References

[1] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965)

[2] A. Cohen et al, Appl. Comput. Harm. Anal. **1**, 54-81 (1993)

[3] L. Genovese et al, J. Chem. Phys. 129, 014109 (2008), BigDFT website: `www.bigdft.org`



Electronic Structure of C_6H_8 with BigDFT code