Wavelets for electronic structure calculations, an introduction and overview

Stefan Goedecker[a]

[a] *Department of Physics, University of Basel*
stefan.goedecker@unibas.ch

Haar wavelets will first be presented to illustrate the basic principles of multiresolution analysis. Then I will introduce three families of wavelets that are useful in the context of electronic structure calculations. Daubechies wavelets have unique properties as a basis set for representing wavefunctions. Interpolating wavelets are very well suited for the solution of partial differential equations, such as Poissons equation. Multiwavelets allow for an easy grid refinement and are therefore well suited to perform all-electron calculations. In addition I will give an overview over several wavelet based libraries of the BigDFT package and some non-standard functionalities of the BigDFt code for exploring potential energy surfaces.

References

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