Wavelet and fractal basis instead plane-wave in ab-initio calculations

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Abstract

The preferred way to solve partial differential equations is to express the solution as a linear combination of so-called basis functions. These basis functions can for instance be plane waves, Gaussians or finite elements (pic.1). Having discretized the differential equation in this way makes it amenable to a numerical solution. In the case of Poisson's equation one obtains for instance a linear system of equation, in the case of Schrödinger's equation one obtains an eigenvalue problem. This procedure is usually more stable than other methods which do not involve basis functions, such as finite difference methods. Wavelets are just another basis set which however offers considerable advantages over alternative basis sets and allows us to attack problems not accessible with conventional numerical methods [1].

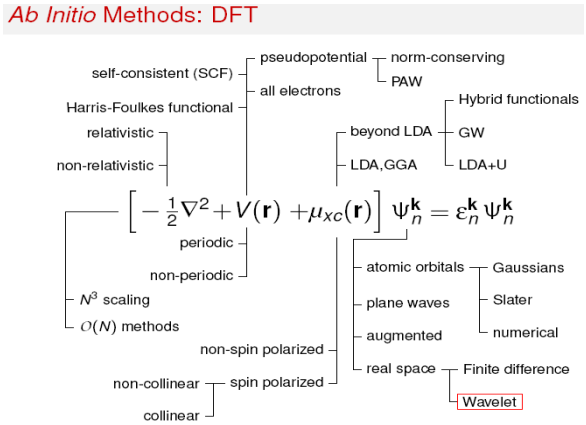
Gaussians and plane waves are at present the most popular basis sets for density functional electronic structure calculations. Wavelets are a promising new basis set that combines most of the theoretical advantages of these two basis sets (pic. 2). They can form a systematic orthogonal basis set that allows for adaptivity, the basis functions being localized both in real (compact support) and in Fourier space.

Using fractal-basis is more effective way for increase quality and speed of calculation than wavelets.

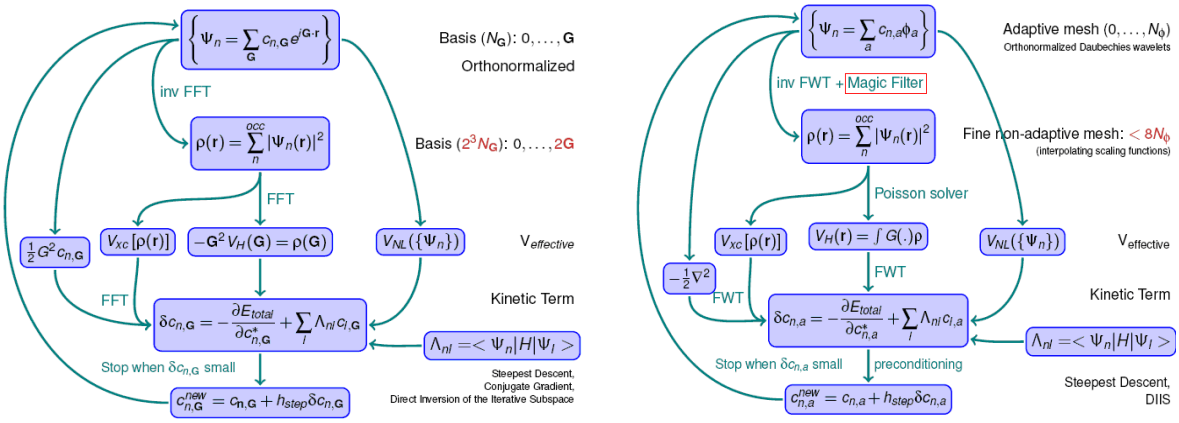
References

[1] S. Goedecker and O. V. Ivanov, Computers in Physics 12, 548 (1998).

Figures



Pic. 1. Using wavelet basis on DFT



Pic. 2. Direct minimization procedure with plane-waves basis (FFT, left) and wavelet basis (FWT, right)