Self-Adaptive Wavelet-Based Electronic Structure Calculations

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The unique properties of a wavelet basis have created an interest in its application to *ab initio* electronic structure calculations. Previous investigations have been limited by the use of a uniform real-space grid for local real-space operations. Furthermore, in many cases the generation of a simple wavelet basis set was carried out prior to, and remained fixed throughout the actual calculations; attempts at an adaptive scheme have been incomplete. In this work, the problem of performing local real-space operations is resolved with the introduction of a generalization of the classic Haar basis. The result is a wavelet-based method which may be multiscale in practice, and not simply in theory. Of equal importance is the approach to the generation of a particular wavelet basis set. Here, a self-adaptive wavelet refinement cycle is incorporated into a traditional iterative method for minimizing the total energy of the system. This allows the generation of an optimal wavelet basis set simultaneously with the solution of the problem. The basis generation is self-adaptive in that it is not directed by any external parameters (e.g., the positions of atoms or chemical bonds) and follows only the information obtained throughout the calculation itself. In comparison to previous wavelet-based calculations, a great deal of flexibility is given to the specific size and configuration of the basis sets which are dynamically generated for each wavefunction.