Adaptive refinement of wavelet based solutions of the Schrödinger equation by independent estimation of the fine resolution coefficients

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Multiresolution analysis (MRA) [1] or wavelet analysis is a successful tool for data compression and it can also be used – similarly to the Fourier analysis – for solving differential equations. Wavelets, the basis functions of MRA, divide the Hilbert space into subspaces, each of which can be characterized by a resolution level index. The wavelet expansion of the functions contain high resolution level wavelets only at those locations, where the function is more rapidly varying, the smoother parts can be expanded by only rough resolution level basis functions. This fact is behind the enormous success of wavelet-based data and image compressing methods, in most of the cases the functions or distributions to be compressed are smooth in most locations, and high resolution is needed only in very restricted domains.

In electron structure calculations the wave functions are usually unevenly detailed, some parts, like the cusps need high spatial resolution to be sufficiently precisely described, while the parts further away from the cores are smooth, they require less fine resolution. According to this fact, and the uniformness of the wavelets, the basis functions of the MRA seem to be successful candidates for basis functions of electron structure calculations [2, 3]. Operators that contain differentiation and multiplications with polynomials can usually be represented in wavelet basis very well[5, 4], the exception is clearly the Coulomb potential. A method is presented here to solve electron structure calculations using wavelets as basis functions, this method automatically adapts to the required resolution level, i.e., it uses higher resolution level basis functions only in those spatial domains, where they are necessary. With the method it is also possible to predict the next, finer resolution level coefficients, if we have a given resolution solution. This property can be used either for estimating the error of the given solution, or for refining it.

[1] Daubechies,I., *Ten Lectures on Wavelets*, CBMS-NSF regional conference series in applied mathematics 61, SIAM, Philadelphia, 1992, p. 176.

[2] Goedecker, S., Ivanov, O. V. *Solid State Commun.*, 105:665, 1998.

[3] Genovese, L., Neelov, A., Goedecker, S., et al. *J. Chem. Phys.*, 129:014109, 2008.

[4] Dahmen, W., Micchelli, C. A., *SIAM J. Numer. Anal.*, 30:507, 1993.

[5] Pipek, J., Nagy, Sz., *J. Comput. Chem.*, 34:460, 2013.