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Publication

An efficient numerical quadrature for the calculation of the potential energy of wavefunctions expressed in the Daubechies wavelet basis

JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

An efficient numerical quadrature is proposed for the approximate calculation of the potential energy in the context of pseudo potential electronic structure calculations with Daubechies wavelet and scaling function basis sets. Our quadrature is also applicable in the case of adaptive spatial resolution. Our theoretical error estimates are confirmed by numerical test calculations of the ground state energy and wavefunction of the harmonic oscillator in one dimension with and without adaptive resolution. As a byproduct we derive a filter, which, upon application on the scaling function coefficients of a smooth function, renders the approximate grid values of this function. This also allows for a fast calculation of the charge density from the wavefunction.