NMTO-like Basis Sets in a Full-Potential Context

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Andersen's development of linear methods, and its realization in the LMTO basis set in particular, has had a profound influence in the electronic structure community. Even while plane wave basis sets have today become dominant, compactness is increasingly important as we work towards large system sizes or try to build in strong correlations. Such basis sets achieve locality by assembling localized wave packets from eigenfunctions which span a certain hilbert space of the original hamiltonian. A big advantage of this scheme is that it can retain accuracy and completeness of original method.

Compactness requires that a basis span a particular hilbert space with a minimal number of orbitals, while at the same time being short range. I will sketch out a scheme that meets these requirements as well as other properties needed for a full-potential framework, such as smoothness of the envelope function, can be realized. Preliminary results on models show that the basis should be comparable to LAPW in accuracy over the physically important energy window, while at the same time being minimal. The basis shares many elements in common with Andersen's NMTO method, such as the possible linearization of an energy-dependent hamiltonian.