Abstract Submitted for the MAR09 Meeting of The American Physical Society

**Compact representations of Kohn-Sham invariant subspaces**<sup>1</sup> FRANCOIS GYGI, University of California Davis, Davis CA 95616 — We present a method to compute a hierarchical approximate representation of the solutions of the Kohn-Sham equations. The approach is based on a recursive bisection algorithm and yields one-particle wavefunctions localized on domains of varying sizes. The accuracy of the representation is set *a priori* by specifying the maximum error in the norm of the approximate wavefunctions. Applications to the electronic structure of large systems are used to illustrate the data reduction achieved by this representation. The achievable data compression is similar to that obtained by truncating Maximally Localized Wannier Functions. Implications for the acceleration of electronic structure calculations and for the development of linear-scaling algorithms will be discussed.

<sup>1</sup>Supported by NSF OCI 0749219 and DOE-SciDAC DE-FC02-06ER25794

Francois Gygi University of California Davis, Davis CA 95616

Date submitted: 20 Nov 2008

Electronic form version 1.4