

Abstract Submitted
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Compact Representations of Kohn-Sham Invariant Subspaces

FRANCOIS GYGI, University of California Davis, Davis CA 95616 — We present an algorithm for the computation of reduced numerical representations of the solutions of the Kohn-Sham equations. The method allows for *a priori* control of the error caused by the reduction process. When applied to Kohn-Sham wavefunctions expanded on a plane-wave basis, this approach leads to a substantial reduction of the size of the datasets used to restart first-principles simulations, with controlled loss of accuracy. Examples of applications to jellium, liquid water and carbon nanotubes will be presented. A comparison with representations in terms of maximally localized Wannier functions will also be discussed.

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