O.4 Generalization of the cRPA scheme : implementation and use. Role of interactions on oxides p orbitals

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The Density Functional Theory (DFT) fails to describe strongly correlated systems. Through times, many methods have been developed to improve this description, such as DFT+U or DFT+DMFT (Dynamical Mean Field Theory). Those methods require an input parameter (U) that characterize the strength of the effective Coulomb interaction between correlated electrons. The cRPA (constrained Random Phase Approximation), is one of the broadly used method to calculate U.

Following Seth *et al.*[1], and based of the previous implementation by Amadon *et al.*[2], we have implemented a new cRPA scheme in `ABINIT`.

The previous implementation was limited to only one strongly correlated orbital per system. Our new version enables the calculation of the effective Coulomb interaction, inside and between any orbitals of a system. These quantities provide a better understanding of the electronic interactions and screening processes at play in strongly correlated systems.

We present here some technical details of the implementation and the way to use it inside `ABINIT`. In addition, we demonstrate some capabilities on a range of actinides dioxides (from UO_2 to CmO_2)[3].

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[1] P. Seth, Ph. Hansmann, A. van Roekeghem, L. Vaugier and S. Biermann, Phys. Rev. Lett. **119**, 056401 (2017)

[2] B. Amadon, T. Applencourt and F. Bruneval, Phys. Rev. B **89**, 125110 (2014)

[3] J.-B. Morée, R. Outerovitch and B. Amadon, Phys. Rev. B **103**, 045113 (2021)