Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Fast response function for finite and bulk systems PETER KOVAL, FEDERICO MARCHESIN, DANIEL SANCHEZ PORTAL, Centro de Fisica de Materiales, Donostia-San Sebastian, Spain (Donostia International Physics Center, Spain), DIETRICH FOERSTER, Laboratiore Ondes et Matiere d'Aquitaine, Bordeaux, France — Many-body perturbation theory of bulk systems is often realized within reciprocal space, using plane-wave (PW) basis sets. PW basis is advantageous because of its elementary basis functions and simple convergence control. However, the number of functions in PW basis grows with third power of unit cell size, irrespective of actual number of atoms present in the unit cell. Moreover, PW basis gives rise to full matrices in tensor algebra due to space-filling nature of PW. An alternative to PW would be usage of localized basis functions. In this contribution, we show how a basis of *dominant products* (DP) can be used to describe excitations in finite and bulk systems. We present calculations of absorption spectra and electron-energy loss spectra within time-dependent density functional theory, realized within DP basis. The usage of localized functions and iterative techniques allow to keep the complexity of the calculations rather low: the overall number of operations grows with third power of number of atoms in the unit cell.Moreover, we have recently shown that Hedin's GW calculations can also be performed using DP basis with an order-N^3 scaling for finite systems. We are currently extending this GW methodology to bulk systems.

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Date submitted: 02 Nov 2012 Electronic form version 1.4