Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

GW without empty states J.A. BERGER, LSI, Ecole Polytechnique and ETSF, L. REINING, F. SOTTILE — The GW approximation (GWA) to the self-energy[1] has proved to be very successful in the calculation of quasi-particle energies for a wide range of solids. However, the GWA is computationally expensive which is mainly due to the slow convergence with the number of unoccupied states that have to be taken into account in its standard sum-over-states expression. In this work we will show that the expression for the GW self-energy can be rewritten explicitly in such a way that no unoccupied states enter. This approach leads to a hierarchy of expressions for the self-energy which converges rapidly. The expressions thus obtained are very simple and can be readily implemented leading to an immediate speedup of GW calculations. Truncation of this hierarchy at lowest order already leads to excellent results for the quasiparticle energies. We use a similar scheme to rewrite the sum-over-states expression for the polarizability such that only occupied states are required.

[1] L. Hedin, Phys. Rev. 139, A796 (1965).

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Date submitted: 20 Nov 2009 Electronic form version 1.4