Abstract Submitted
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Local and non-local vertex corrections in GW for extended and localized systems[1] MARTIN STANKOVSKI, ANDREW MORRIS, BENJAMIN ROBINSON, REX GODBY, University of York, KRIS DELANEY, UIUC Urbana, PATRICK RINKE, Fritz-Haber-Institut Berlin, ULF VON BARTH, CARL-OLOF ALMBLADH, University of Lund, PABLO GARCÍA-GONZÁLEZ, UNED Madrid — A non-local operator like the self-energy can be consistently calculated through many-body perturbation theory for systems of interacting electrons. This is usually done within the framework of Hedin's GW approximation. If the initial Green's function is obtained within a local approximation like DFT-LDA, there is in principle a local vertex given by the static exchange-correlation kernel in the first iteration (Del Sole *et al.* PRB **49**, 8024 (1994)). We present total energies and bandwidths for jellium and equivalent quantities for He, Be and Ne. We show that a local vertex implemented in both the screened interaction and the self-energy leads to unphysical results. A local vertex in the screened interaction only provides results on par with or slightly better than standard one-shot G_0W_0. Finally, we obtain significant improvements by introducing non-local vertex corrections derived from non-local starting aproximations for the self-energy.

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