Local and non-local vertex corrections in GW for extended and localized systems

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— 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 approximations for the self-energy.

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