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**GW quasi-particle spectra without sums over empty states** PAOLO UMARI, CNR-INFM Democritos, Trieste, Italy, STEFANO BARONI, SISSA & CNR-INFM Democritos, Trieste, Italy — We introduce a method that allows for the calculation of quasi-particle spectra in the GW approximation, yet avoiding any explicit reference to empty one-electron states. This is achieved by expressing the irreducible polarizability operator and the self-energy operator through a set of linear response equations, which are solved using a Lanczos-chain algorithm. We first validate our approach by calculating the vertical ionization energies of the benzene molecule and then show its potential by addressing the spectrum of a large molecule such as free-base tetraphenylporphyrin and those of some glassy materials.

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