The Quasiparticle Self-Consistent $GW$ Approximation
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A new type of self-consistent scheme within the $GW$ approximation is presented, which we call the quasiparticle self-consistent $GW$ (QS$GW$) approximation. It is based on a kind of self-consistent perturbation theory, where the self-consistency is constructed to minimize the perturbation. QS$GW$ describes optical properties in a wide range of materials rather well. Self-consistency dramatically improves agreement with experiment, and is sometimes essential. QS$GW$ handles both itinerant and correlated electrons on an equal footing, in a true $ab$ $initio$ manner without any ambiguity about how a localized state is defined, or how double-counting terms should be subtracted. Thus QS$GW$ combines advantages separately found in many kinds of $ad$ $hoc$ extensions to the LDA (e.g. LDA+$U$ theory), in a simple and fully $ab$ $initio$ way. QS$GW$ avoids some formal and practical problems encountered in conventional self-consistent $GW$, and also LDA-based $GW$ approximations, which will be discussed.

Weakly correlated materials such as Na and $sp$ semiconductors are described with uniformly high accuracy; QS$GW$ also reliably treats many aspects of correlated materials. Discrepancies with experiment are generally small and systematic, and depend in a regular way on the degree of localization of the electronic states. Most of the discrepancy can be explained in terms of omission of short-ranged excitonic contributions to the irreducible polarization function calculated in the RPA. Its consistently high accuracy make QS$GW$ a versatile method that can reliably predict many kinds of materials properties in a unified framework, for example, critical energy-band parameters in InN and CuInSe$_2$, the spin wave spectra in Fe and NiO, and a reasonable description of a number of $4f$ compounds such as ErAs. GdN is predicted on the cusp of a new kind of first-order metal-insulator transition.