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 (QSGW) approximation. It is based on a kind of self-consistent perturbation theory, where the self-consistency is constructed to minimize the perturbation. QSGW describes optical properties in a wide range of materials rather well. Self-consistency dramatically improves agreement with experiment, and is sometimes essential. QSGW 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 QSGW 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. QSGW 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; QSGW 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 QSGW 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.