Quasiparticle self-consistent GW

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We present some progress in the development of a semi self-consistent GW method based on the all-electron, full-potential LMTO method. Starting from a trial one-body Hamiltonian H_0 (or bare Green function G_0), we can get the self-energy $\Sigma(\omega)$ and also the Green function G in the usual GW calculation. Then we can define new one-body Hamiltonian H_0' by fixing the energy-dependence of $\Sigma(\omega)$ (we tested some possibilities), so that H_0' can well reproduce the quasiparticle (QP) part contained in G. Here we require $H_0 = H_0'$, so as to determine H_0. This is a self-consistentcy requirement taken as **"non-interacting Hamiltonian $\approx$ QP part of G"**. Thus we call our method as QPscGW . This is a kind of self-consistent perturbation thoery.

This H_0 gives "the *best* bare QP picture", which get to be the independent-particle picture for the weakly-correlated systems. Then QPscGW gives directly the QP density of states (QP-DOS) in the sense of independent-particle picture, which can be justified by the Landau's Fermi liquid theory. The QP bands given by H_0 can be used directly within the independent-particle picture to evaluate quantities, e.g. response functions, transport, and so on.

The "bare QP picture" should be also a rigid starting point even when we try to go beyond the independent-particle picture. The method may be viewed as a way construct the most suitable quadratic part of the full Hamiltonian for many-body perturbation theory. As for the spectrum DOS (SP-DOS), the imaginary part of the full Green function G, it can be calculated by a one-shot GW calculation (or GW +extensions) from the QPscGW result.

This situation is in contrast with the full self-consistent GW method (full scGW), which makes SP-DOS self-consistent. Compared the full scGW, QPscGW is advantageous in two ways:
(1) Numerically easier and more stable. We successfully applied it to wide range of materials.
(2)There is self-consistency in both the QP bands and the dynamically screened Coulomb interaction W (they are obtained at the same time). By contrast, the full scGW give problematic W, which results in poor G.

We applied our QPscGW to metals, semiconductors, oxides, magnetic materials, f-electron materials (in progress) and so on. Our results show very systematic improvement over LDA compared with experiments. We present two key findings:
(1) large improvements are found for materials where one-shot GW fails.
(2) The discrepancies with experiment are very systematic, and can be explained in terms of what GW theory omits from the exact hamiltonian.
As for semiconductors, not only band gaps but many other properties are improved, such as effective mass. For NiO and MnO, *d-d* splitting and relative positions of oxygen $2p$ bands move closer to experimental results. Transition metals show a small, systematic d-band width narrowing relative to LDA. We also present recent results for MnGaAs and half-metallic compounds.

Finally, we report some progress on attempts to compute the total energy in RPA without the LDA kinds of approximations.

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