Quasiparticle Self-consistent GW Approximation as a Framework for Many-body Hamiltonians

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As is well known, parameters U and J entering into the LDA+U and LDA+DMFT Hamiltonians matrix elements of the screened coulomb interaction W, subject to a constraint to avoid double-counting of self-screening. In any case U and J are constructed in practice in the time-dependent Hartree approximation. Moreover, there are manifold ambiguities inherent in the manner in which U and J are made. Usually U is taken in the static limit, $U{\approx}U(\omega{=}0)$. Finally, the framework, LDA or DFT, which $+U$ or +DMFT improve upon, cannot be regarded as merely a lower order approximation, resulting in further ambiguities. The auxiliary one-electron hamiltonian that is a by-product of DFT, generates fictitious eigenvalues that are nevertheless assumed to be quasiparticle spectra that LDA+U or LDA+DMFT corrects.

Here we show how the quasiparticle self-consistent GW approximation (QSGW), sheds light on many of the approximations and assumptions inherent in models like LDA+DMFT, and in GW itself. GW is a low-order perturbation theory, which makes the time-dependent Hartree approximation for W. As with LDA+U and LDA+DMFT, GW is usually built around the LDA ($G^{\rm LDA}W^{\rm LDA}$) and has its own ambiguities. We show QSGW is an optical choice for GW, and circumvents many of the ambiguities and shortcomings of $G^{\rm LDA}W^{\rm LDA}$. QSGW describes optical properties in a wide range of materials rather well, e.g. it reproduces the low-energy ARPES spectra in Fe within the experimental resolution. Self-consistency dramatically improves agreement with experiment, and is sometimes essential. It handles both itinerant and correlated electrons on an equal footing, without any ambiguity about how a localized state is defined, or how double-counting terms should be subtracted.

Discrepancies with experiment in the quasiparticle spectra are small and systematic, and can be identified with the vertex omitted from W. Thus QSGW provides the optimal framework for determining the limits to the RPA. We find, for example that $W^{\rm RPA}(\omega{=}0)$ is systematically overestimated in insulators, by a universal factor of about 5/4. Finally, we show that nonlocality, missing from LDA+U and LDA+DMFT theory, is not small. At least in the Fermi liquid regime of $BaFe_2As_2$, the self-energy can be well separated into (static, non-local) + (dynamic, local) contributions.