Effective interactions in many-body perturbation theory

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Many-body perturbation theory is usually formulated in terms of a screened, instead of the bare Coulomb interaction. There is, however, no unique prescription for what this screened interaction should be. This is one of the reasons for the many different flavors that can be found in ab initio calculations, for example, for Hedin's GW approximation [1] for the self-energy. In this talk we will analyze the situation and give arguments for certain choices, both for the calculation of spectroscopic quantities and for the total energy. These choices can be formulated in terms of approximate vertex corrections to the GW expression, where W is defined to be the exact test charge-test charge screened interaction [2]. We then broaden the concept of the screened interaction to a generalized effective interaction, for which we derive in principle exact equations as well as promising approximations. We show that this allows one to go beyond the GW approximation in an efficient way, avoiding the computational complexity of full vertex corrections. A further way to speed up the calculations will also be introduced. Illustrations include quasiparticle energies, full spectral functions and total energies for model systems and real materials.

[1] Lars Hedin, Phys. Rev. **139**, A796 (1965)
[2] Abdallah El Sahili, Francesco Sottile and Lucia Reining, Journal of Chemical Theory and Computation **20**, 1972 (**2024)**