Bethe-Salpeter equation for correlation energies and post-GW self-energies

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To describe materials properties, the two particle propagator of many-body perturbation theory is a key quantity. Once calculated, it allows one to determine particle conserving excitation energies, correlation energies, as well as charge neutral quasi-particle energies, such as band gaps.

To calculate the two particle propagator the Bethe-Salpeter equation (BSE) is usually discretized in a particle-hole basis allowing for efficient computations. To access the quantities enumerated above, however, one needs to go beyond the usual Tamm Dancoff approximation, which is done in the present work.

Using this approach we calculate the correlation energy of the homogeneous electron gas. Furthermore, we construct from the two-particle propagator the self-energy operator, allowing us to go beyond the random phase approximation and the standard GW scheme respectively. The relevance of this post-GW self-energy contribution is calculated for the homogeneous electron gas and for prototypical semiconductors and insulators.