Ab-initio description of semiconductors and nanocrystals

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Linear optical properties can be accurately calculated using the Bethe-Salpeter equation for the polarization function. After introducing a suitable product basis for the electron-hole pairs, the Bethe-Salpeter equation is usually recast into a complex non Hermitian eigenvalue problem that is difficult to solve using standard eigenvalue solvers. In solid state physics, it is therefore common practice to neglect the problematic coupling between the positive and negative frequency branches reducing the problem to a Hermitian eigenvalue problem (Tamm-Dancoff approximation). We use time-inversion symmetry to recast the full problem into a quadratic Hermitian eigenvalue problem, which can be solved routinely using standard eigenvalue solvers even at a finite wave vector. This allows us to access the importance of the coupling between the positive and negative frequency branch for prototypical solids.

However, within the product basis of two-orbital states, the resulting matrix of the corresponding BSE eigenvalue problem can be solved numerically efficient only for matrix sizes up to 100.00-150.000. As an alternative approach, we have exploited a real time evolution of orbitals. Applying an infinitely short electric field in time and then following the evolution of the electron orbitals and the evolution of the dipole moments, the long wavelength response function is obtained by the Fourier transformation of the time evolved dipole moments.

In the context of time-dependent denstiy functional theory, this time evolution method is equivalent to the Casida approach. The latter one yields an algebraic eigenvalue problem, formally very similar to that of the Bethe-Salpeter equation. We compare the results and performance of these two approaches for the projector augmented wave method. To allow for large time steps and still rely on a simple difference scheme to solve the differential equation, we correct for the errors in the frequency domain, using a simple analytic equation. In general, we find that both approaches yield virtually indistinguishable results. For standard density functionals, the time evolution (TE) approach is, with respect to the computational performance, clearly superior compared to the solution of the Casida equation. However, for functionals including nonlocal exchange, the direct solution of the Casida equation is usually much more efficient, even though it scales less beneficial with system size.