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Many-Body Perturbation Theory and Density-Functional based approaches: successful combinations

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Today, in the framework of solid state physics two main ab initio approaches are used to describe ground- and excited state properties of condensed matter: on one side, static ground state density functional theory (DFT) and its time-dependent extension (TDDFT) for the description of excited states; on the other side, Many-Boby Perturbation Theory (MBPT), most often used in Hedin s GW approximation [1] for the electron self-energy, or the Bethe-Salpeter equation for the calculation of response functions. Both approaches have led to breakthroughs, but suffer from different shortcomings: MBPT has a relative conceptual clarity and therefore allows one to find good approximations, but calculations are in general numerically very demanding. DFT-based approaches are in principle computationally more efficient, but a generally reliable and at the same time efficient description of exchange-correlation effects within TDDFT is difficult to obtain. In recent years a major effort has therefore been made in order to combine MBPT and TDDFT, searching for a formulation that would keep the advantages of both approaches (see e.g. [2,3]). In this talk we will discuss different ways to derive a linear response exchange-correlation kernel for TDDFT from MBPT. The strength of various approximations, that have been shown to reproduce continuum and bound excitons for a wide range of materials, as well as possible problems will be outlined, and the computational efficiency of the method examined. The question of how to use such a combination of MBPT and TDDFT in order to obtain vertex corrections to the self-energy [4] will also be addressed.

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