Time-dependent density functional theory: design and use of exchange-correlation kernels

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Abstract: Time-Dependent Density Functional Theory (TD-DFT) is an in principle exact approach to calculate the evolution of the electron density of a system under the influence of a time-dependent external potential. As a consequence, in linear response it yields the in principle exact density-density response function. However, in practice many observations cannot be described and understood on the basis of currently used approximate functionals. In particular, in extended systems much effort is devoted to the design of the so-called exchange-correlation kernel, which is the variation of the exchange-correlation potential with respect to the density. Two of the open problems are the description of excitonic effects, and the inclusion of double or higher excitations, such as double plasmons. In this seminar we will discuss two main directions to design kernels that can overcome some of the problems of the state-of-the-art approximations. One direction explores the possibility to perform advanced calculations in a model system and to design a procedure that we call ``connector'', which allows us to use the results of the model in order to calculate spectra in real systems. We will discuss the principles and general properties of such an approach, and look at inelastic x-ray scattering spectra as an illustrative example [1]. The second strategy is to learn from many-body perturbation theory, based on Green's functions. Ultimately, the two approaches might be combined into a single powerful scheme. Finally, we will turn the second strategy around and discuss to which extent we can use TDDFT to correct current approximations in the framework of many-body perturbation theory.

[1] M Panholzer, M Gatti, L Reining; Phys. Rev. Lett. 120, 166402 (2018).

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