Progress in time-dependent density functional theory for excited states

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Résumé

The Runge-Gross extension of the Hohenberg-Kohn theorems to time-dependent external potentials opened a route to extract in principle exact excited state properties from the time-dependent density. The equivalent Kohn-Sham formulation for time-dependent problems stuffs all the complexity of the N-body problem into a time-dependent exchange-correlation (td-xc) functional, which is unknown as the ground-state counterpart. The td-xc functional depends on the densities at all times (memory), introducing thus a "time-dependence" of the exchange-correlation effects. The popular "adiabatic approximation" to the td-xc functional, which avoids whatsoever memory effects, is known to fail even qualitatively for representing strong correlation in excited states. Several memory td-xc functionals derived using many-body perturbation theory can describe excited-state correlation better. However, is the memory in the td-xc functional unavoidable or an artifact of the formulation? In this talk, I will discuss the meaning of "memory" from the perspective of time-dependent density response.

Mots-Clés: density functional theory, time, dependent density functional theory, excited states, linear response

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