Surprises with Mean Field Dynamics

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We investigate the depletion of single-electron states in small molecules under the influence of very short XUV pulses. The system is described by an effective mean field theory coined Time Dependent Density Functional Theory which bears strong similarities with the usual Time Dependent Hartree Fock approach to nuclear dynamics. Calculations to analyze the dynamics rely on real time Time Dependent Density Functional Theory (TDDFT) using the QDD (Quantum Dissipative Dynamics [1]) and EDAMAME ((Ehrenfest DynAMics on Adaptive MEshes) code [2] packages.

For *some* XUV energies we observe a marked occupation inversion, where depletion of the deep bound state becomes much larger than other ones. This drives a dipole instability, i.e. a spontaneous reappearance of the dipole signal long after the laser pulse is over and the dipole signal has died out. The dipole signal that emerges from this instability can be identified as a particular low-energy structure in photo-electron spectra. This instability can be explored simplifying the excitation mechanism by instantaneous generation of a hole in one of the occupied states of the system. We investigate how the dipole instability depends on the system, the state in which the hole is cut, and the amount of depletion which is given to the hole state. The mechanism might appear in other systems described by mean field approaches. We show some examples taken from the well-known Lipkin-Glick-Meshkov models as well as from comparable spin models.

References

[1] P.M. Dinh, M. Vincendon, F. Coppens, E. Suraud, P.-G. Reinhard, *Computer Phys. Comm.* **270** (2022) 108155.

[2] D. Dundas, *J. Chem. Phys.* **136** (2012) 194303.

[3] P.-G. Reinhard, D. Dundas, P.M. Dinh, M. Vincendon, E. Suraud, *Phys. Rev. A Lett*. **107** (2023) L020801.

[4] P.-G. Reinhard, P.M. Dinh, D. Dundas, M. Vincendon, E. Suraud, *Eur. J. Phys. Special Topics* **232** (2023) 2095, special issue on "Ultrafast Phenomena from attosecond to picosecond timescales : theory and experiments".

[5] D. Hughes, D. Dundas, P.M. Dinh, M. Vincendon, P.-G. Reinhard, E. Suraud, *Eur. Phys. J. D* **77** (2023) 177.