

2nd March 2017 - 16:00h

CFEL – Building 99, seminar room I+II (ground floor)

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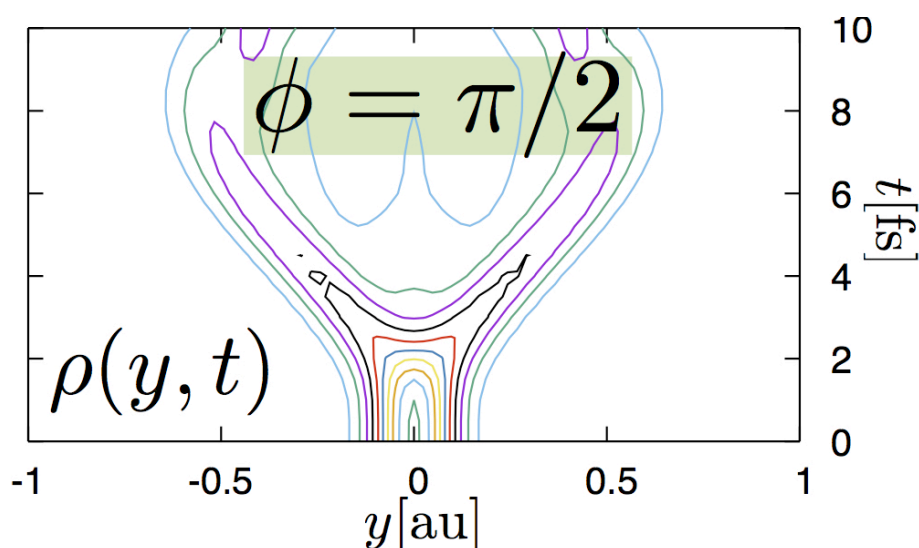
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Coupled nuclear and electronic dynamics in molecules

The transfer of electrical charge on a microscopic scale is very often related to electron or proton displacements supported by molecules, biological structures and materials. Femtosecond lasers have a long history of being used to trigger, probe and steer these kinds of dynamics, where the usual paradigm is that of an optical electronic excitation leading to coherent nuclear wavepacket dynamics on the potential energy surfaces of excited electronic states followed by the eventual relaxation back to the ground electronic state.

Besides the generation of nuclear wave packets, the advent of ultrashort, broadband lasers with pulse durations in the attoseconds to few femtoseconds range makes it now possible to launch coherent superpositions involving two or more electronic states. The electronic and nuclear dynamics initiated by the laser pulse become now intermingled in a more complex manner as compared to the dynamics started in a single electronic state.

In this seminar we will see examples in which the coupled evolution of the nuclear and electronic degrees of freedom strongly influences the time evolution of the system [1,2,3] and especially its electronic coherence properties [4]. We will have an outlook on how electronic superpositions can affect the motion of the nuclei in molecules and how some degree of control could be achieved based on such effects.



[1] Z. Li, M. E. Madjet, OV and R. Santra, Phys. Rev. Lett. 110, 038302 (2013)

[2] H. Timmers, Z. Li et al., Phys. Rev. Lett. 113, 113003 (2014)

[3] Z. Li, OV and R. Santra, Phys. Rev. Lett. 115, 143002 (2015)

[4] C. Arnold, OV and R. Santra, Phys. Rev. A, accepted (2017)