

Self-consistent 2D-Bohmian description of photoelectron holography

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Synopsis We have developed a self-consistent 2D-approach to quantum description of electron dynamics in strong fields, based on the hydrodynamical Bohmian formulation of quantum mechanics. We implement our approach to photoelectron holography in diatomic molecules, allowing to picture the experimental results of Meckel *et al.*[4] in terms of quantum trajectories.

D. Bohm has introduced in 1952 a reformulation of the time dependent Schrödinger equation (TDSE) based on an hydrodynamic treatment of the electron flux. One of the main interests of this approach is to give access to quantum electron trajectories during the interaction, which facilitates experimental interpretations. These electron trajectories can be obtained subsequently to a former (and standard) TDSE calculation. This constitutes the *analytical way*. However it is also possible to integrate directly the quantum Bohmian equations of motion. This is the *self-consistent approach*, that we describe and employ here.

The self-consistent approach is appealing since it does not present the limitations of standard TDSE integrations related to basis set convergence, prohibitive size of lattice grids,... The Bohmian approach employs a Lagrangian formulation of probability flow, which is computationally advantageous and can be easily generalized to multi-center problems. However it is known to be difficult to implement, because of numerical instabilities related to formation of nodes in wavefunctions. We have succeeded in circumventing these problems[5], extending 1D-recipes[2, 3] to multi-dimensional problems.

Details on practical solutions to integrate the hydrodynamical equations of motion will be given at the Conference. However we already employed our approach to picture the experimental observations of Meckel *et al.*[4] concerning electron holography in N₂ molecules. In the experiment, aligned N₂ molecules are ionized by a linearly polarized, strong and short laser pulse. Interference patterns then show up in the photoelectron spectra, depending on the angle between laser polarization and molecular alignment direction. Model calculations attributed these features to the shape of the ionizing wavepacket at time of ionization[4].

We have applied our Bohmian approach to simulate the experiment, in the framework of the single active electron approximation. The photoelectron angular distribution, including interference patterns, are nicely reproduced. Beyond this, our simulations allow to follow the dynamics of the elec-

tron wavepacket throughout the interaction in terms of trajectories. These latter clearly show that as soon as the molecule is neither parallel nor perpendicular to the pulse polarization, an offset of the ionizing wavepacket appears as the electron leaves its parent molecule, leading finally to a photoelectron distribution which is not symmetric with respect to the polarization direction. This is illustrated in Fig. 1 in cases of molecules aligned at 45 and 90° with respect to the laser field. This quantum picture confirms directly the interpretation of [4]. An in-depth analysis of the results will be presented at the Conference.

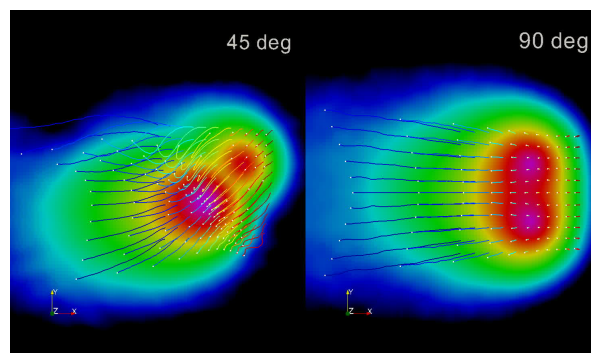


Figure 1. Snapshot of electron density after ionization of N₂ molecules aligned at 45° (left) and 90° (right) with respect to laser polarization.

Furthermore, we will illustrate how the nuclear vibration influences the electron dynamics, beyond the usual Born-Oppenheimer approximation. The hydrodynamical approach is particularly well suited to study non-adiabatic dynamics.

References

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