Non-sequential double ionization of one-dimensional He by effective potentials of natural spin-orbitals

([1]*Graduate School of Arts and Sciences, The University of Tokyo,* [2]*School of Science, The University of Tokyo*) ○Naoki Negishi[1], Tsuyoshi Kato[2], Kaoru Yamanouchi[2]

Keywords: *intense laser field, electron correlation, time-dependent many-body theory, one-electron picture, electron rescattering*

When a He atom is exposed to an intense near-infrared laser field whose intensity is in the range of 0.1–1.0 PW/cm^2, the double ionization into He^{2+} proceeds very efficiently so that the yield of He^{2+} is larger by more than 10^7 times than that predicted based on the single active electron approximation [1]. This enhancement of the double ionization process of He has been intensively studied in the past few decades, and it has been revealed that the electron correlation plays an important role in the double ionization process, in which two electrons are ejected in a non-sequential manner.

In the present study, in order to examine the mechanism of the non-sequential double ionization (NSDI) of He proceeding in the course of the interaction with an intense laser field within the framework of the multi-configuration time-dependent Hartree-Fock (MCTDHF) method [2], we introduce a time-dependent complex-valued effective potential for the time-dependent natural spin-orbitals (NSOs) with the time dependent occupation numbers, so that we can describe the correlated motion of electrons in terms of a single-electron picture. We perform numerical calculations of a one-dimensional He atom exposed to a three-cycle pulse at 750 nm and found that one term appearing in the imaginary part of the effective potential increases or decreases the NSO density depending on its sign varying as a function of the electron coordinate.

Indeed, at the rescattering time of t = 4.5 fs, the result of the calculation shows that the orbital density of the highest occupied natural orbital (HONO) is decreased in the coordinate range in which the imaginary part of the effective potential of HONO takes a large negative value and that the orbital density of the other orbitals like HONO+3 is increased in nearly the same coordinate range. This increase in the orbital density of the HONO+3 can be regarded as the result of the transfer of the orbital density from the HONO.

The result of the MCTDHF calculation above shows that, within the single-electron picture, we can interpret the NSDI of He in terms of the orbital densities, which are transferred between the bound natural orbitals and the high-energy natural orbitals.

References:

[1] B. Walker, B. Sheehy, L. F. DiMauro, P. Agostini, K. J. Schafer, and K. C. Kulander, *Phys. Rev. Lett.* **73**, 1227 (1994).

[2] T. Kato and H. Kono, *Chem. Phys. Lett.* **392**, 533 (2004).