Siegert-state method for ionization of molecules in strong field

Linda Hamonou*[1], Toru Morishita*[2], Oleg I. Tolstikhin†[3], and Shinichi Watanabe*[4]

*Department of Engineering Science, The University of Electro-communication, Tokyo, Japan
†Russian Research Center "Kurchatov Institute", Kurchatov Square 1, Moscow 123182, Russia

Synopsis Our purpose is to create a numerical method able to study the ionization processes in molecular systems by strong field by calculating the Siegert states energies and associated ionization rates which are solutions to the stationary Schrödinger equation satisfying the regularity and out-going-wave Siegert boundary conditions. We present energies and ionization rates obtained for H_2^+.

Over the past few decades, ionization processes in atoms and molecules by intense laser field have been extensively investigated both theoretically and experimentally. More precisely, in molecular cases the orientation or alignment dependence of the ionization rates to strong electric field has been proven fundamental to understand strong field interaction with molecular systems such as rescattering processes including high-order harmonic generation (HHG), high-energy photoelectron spectra, etc [1]. While the MO-ADK model [2] has been widely used to estimate the ionization rates for various systems, it is known to reach a limit in relatively weak field in the tunneling regime, therefore a new theory is needed to improve the accuracy of ionization rates obtained and the understanding of the physical processes involved.

We have recently established a theoretical and computational method to calculate accurate ionization rates and energies of atoms in a static electric field by solving the time-independent Schrödinger equation [3]. It is shown that the complex quasi-energies (energy shift and ionization rates) as well as the transverse momentum distribution for the outermost electron of rare gaze atoms can be calculated efficiently and accurately in the over barrier regime as well as in the tunneling regime. In this present abstract we present the extension of the Siegert-state method to be applied to simple diatomic molecular systems. We solve the stationary Schrödinger equation and construct complex eigen solutions satisfying the Siegert boundary conditions in parabolic coordinates using the R-matrix theory. The space is then divided in two regions: In the inner region, the R-matrix basis is obtained using slow variable discretization (SVD) method [4], while in the outer region, the molecular potential is replaced by a purely coulomb tail allowing the problem to become separable in parabolic coordinates and reducing it to find the solutions to uncoupled equations. The complex quasi-energies are obtained by matching the inner region R-matrix with the outer-region solutions. The stationary Siegert states obtained can be used to extend a newly developed adiabatic theory [5] of ionization of molecules by intense time-dependent laser field.

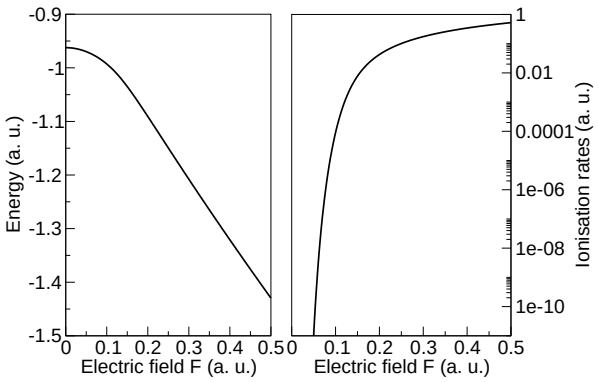

Figure 1. Energy and ionization rates for a model H_2^+ molecular ion as a function of electric field F. The molecule is aligned with the electric field.

References

[1] T. Morishita, A.-T. Le, Z. Chen and C. D. Lin, Phys. Rev. Lett. **100**, 013903 (2008)

[2] X. M. Tong, Z. X. Zhao and C. D. Lin, Phys. Rev. A **66**, 033402 (2002)

[3] P. A. Batishchev, O. I. Tolstikhin and T. Morishita, Phys. Rev. A **82**, 023416 (2010)

[4] O. I. Tolstikhin, S. Watanabe and M. Matsuzawa, J. Phys. B **29** L389 (1996)

[5] O. I. Tolstikhin, T. Morishita and S. Watanabe, Phys. Rev. A **81**, 033415 (2010)

[1] E-mail: linda@power1.pc.uec.ac.jp [2] E-mail: toru@pc.uec.ac.jp [3] E-mail: olegabroad@mail.ru [4] E-mail: shin@pc.uec.ac.jp