Analysis of strong-field enhanced ionization of molecules using Bohmian trajectories

Ryohto Sawada[1,2], **Takeshi Sato**[2] **and Kenichi L. Ishikawa**[1,2]

[1] *Department of Applied Physics, Graduate School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

[2] *Photon Science Center, Graduate School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

sawada49@atto.t.u-tokyo.ac.jp

Abstract: We investigate strong-field enhanced ionization of 1D hydrogen molecule using Bohmian trajectories. Contrary to the common belief, we find that the electron ejections both from the down- and up-field atoms are comparably important.

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The ionization dynamics of atoms and molecules in intense femtosecond laser pulses is of great interest in a variety of fields such as attosecond science and coherent control of chemical reactions. It is widely accepted that the ionization probability of molecular ions depends on internuclear distance and strongly peaks at a critical distance larger than its equilibrium value. A commonly accepted mechanism of this phenomenon called enhanced ionization is depicted in Fig. 1 (a) [1]. Around the critical distance (middle panel), the electron begins to localize in each potential well. Then, the electron in the up-field well can easily ionize through the inner barrier directly to the continuum. The genuineness of this view is, however, still under debate and a subject of active research [2].

In this work, we address the mechanism of enhanced ionization using Bohmian trajectories [3] with which we can clearly visualize the flow of the electron wave packet, by analogy to classical flow visualization with, e.g., fluorescent beads. Since the Newton-like equation of motion for each Bohmian trajectory contains the quantum potential, a whole set of trajectories convey the information completely equivalent to the wave function unlike a classical analysis.

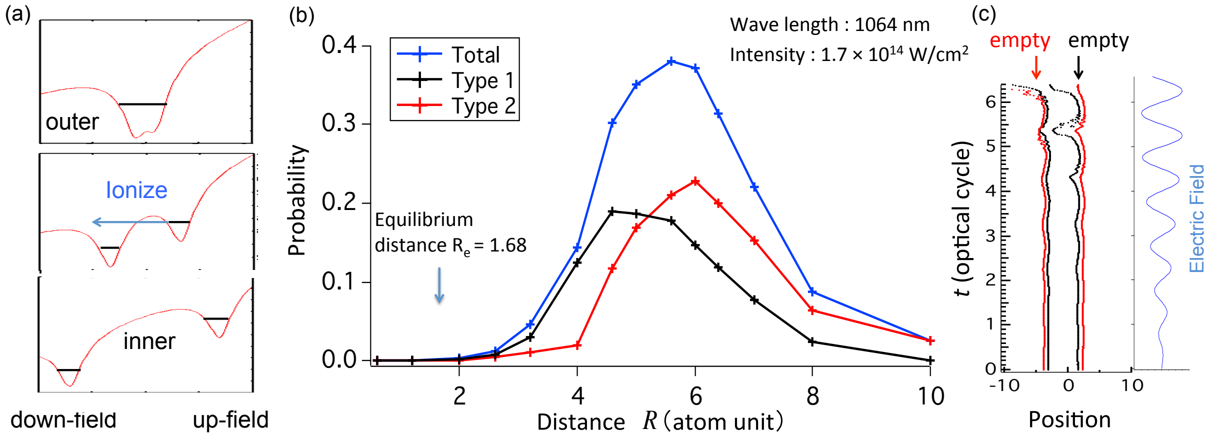

Fig. 1. (a) Commonly accepted mechanism of enhanced ionization. (b) Total (blue) ,Type 1 (black) and Type 2 (red) ionization probabilities. (c) Typical examples of Type1 (black) and Type 2 (red) ionizing trajectories.

We consider the one-dimensional model for H_2 in which two protons are fixed on the x-axis and the electronic motion is restricted along this axis. The field-free Hamiltonian is given as :

$$H = -\frac{1}{2}\sum_{i=1}^{2}\left[\frac{d^2}{dx_i^2} - \frac{1}{\sqrt{\left(x_i \pm \frac{R}{2}\right)^2 + \alpha}}\right] + \frac{1}{\sqrt{(x_1 - x_2)^2 + p}} \quad (1)$$

where R denotes the internuclear distance, and p = 1.2375 and α= 0.7 are the soft Coulomb parameters [4]. The laser wavelength and intensity are assumed to be 1064 nm and 1.7×10^{14} W/cm^2 with a 5-cycle ramp-up, respectively [Fig. 1 (c)]. We numerically solve the time-dependent Schrödinger equation and each Bohmian trajectory is obtained by numerically integrating the equation of motion for a given initial position $(x_1(0), x_2(0))$, with the quantum potential $Q(x_1,x_2,t) = \sum_{i=1}^{2} -(\partial^2 A(x_1,x_2,t)/\partial x_i^2)/2A(x_1,x_2,t)$ derived from the instantaneous wave function where A is real amplitude of the wave function.

In the blue curve in Fig. 1 (b), we show the ionization probability P as a function of internuclear distance R. Our analysis identifies two classes of ionizing whose typical examples are shown in Fig. 1 (c). In Type 1 ejection, tunneling through the inner barriar happens and both of the electrons are around the down-field core just before the ionization. Since the right (up-field) core is empty after the ionization, this type would be observed as *ionization from the up-field core* in experiments. In Type 2, on the other hand, tunneling through the inner barriar never happens. This type, hence, would be observed as *ionization from the down-field core*. Comparing the ionization probability of each type [black and red lines in Fig. 1 (b)], we find the ejection from the down-field core contributes significantly as well although the ionization from the up-field core has been often highlighted as a mechanism of the enhanced ionization [1, 2].

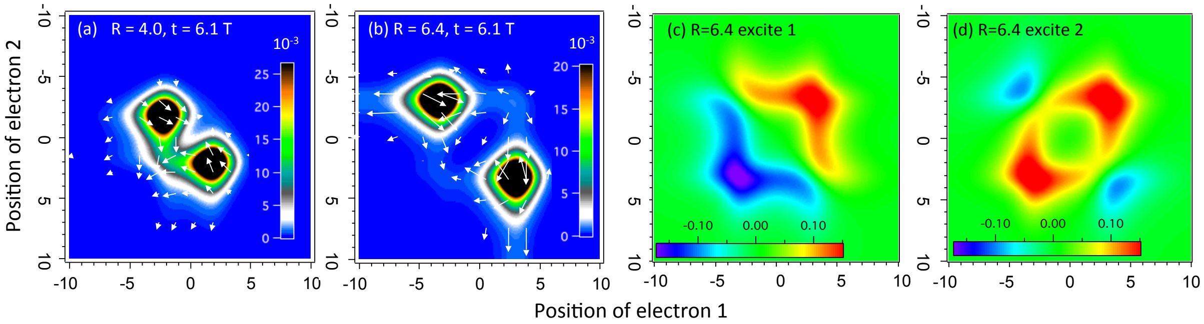

Fig. 2. (a,b) The electron density (color plot) and the particle current density (arrow) at $t = 6.1\,T$ for (a) $R = 4$ and (b) 6.4 a.u. (c,d) Wave function of the (c) first and (d) second excited states at $R = 6.4$. The electric field (force acting on the electrons) is in the positive (negative) direction.

Then, why is the ejection from the down-field core also enhanced? To address this question, we plot the particle current density $\vec{j} \equiv \frac{i}{2}(\psi\nabla\psi^* - \psi\nabla\psi^*)$ and electron density at $t = 6.1\,T$, with T being the optical cycle in Fig. 2 (a) and (b) for $R = 4$ and 6.4 a.u., respectively. At $R = 4$a.u., most of the currents are directed to the lower-left region which favors subsequent type 1 ionization. At $R = 6.4$a.u., on the other hand, we see more current at $x_1(x_2) \sim 3$a.u. and $x_2(x_1) < -7$a.u., undergoing type 2 ionization. The trend in Fig. 2 (a) and (b) can be roughly explained as a superposition of the first and second excited states [Fig. 2 (c,d)]. Their populations have peaks around critical internuclear distance [5]. General forms of the particle current density can be reproduced by superposing these two states with the same ($R = 4$) and opposite ($R = 6.4$) phases, respectively. Thus, the excitation of multiple states leads to either type 1 or 2 ionization, depending on their phase difference.

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