Tunneling dissociation of H_2^+ and its isotopes in THz laser pulses

Zhi-Chao Li,[1] Camilo Ruiz,[2] and Feng He[1,3,*]

[1]*Key Laboratory for Laser Plasmas (Ministry of Education) and Department of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, People's Republic of China*

[2]*Grupo de Investigación en Óptica Extrema, Universidad de Salamanca, E-37008 Salamanca, Spain*

[3]*State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai 200062, China*

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Tunneling ionization of atoms and molecules plays a major role in strong field physics. In this paper we study the nuclear version of this phenomenon: tunneling dissociation of H_2^+ and its isotopes in the interaction with THz pulses. We show strong evidence supporting the concept of tunneling dissociation by numerically solving the time-dependent Schrödinger equation (TDSE). In our simulations, we observe a significant dissociation probability as a function of the driving field compatible with tunneling dissociation. We also observe nuclear rescattering, which induces high nuclear momenta, in clear analogy to the electron rescattering, which is very important in strong-field physics. This study offers an alternate perspective on the molecular tunneling dissociation in long-wavelength laser fields.

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I. INTRODUCTION

One of the most fundamental physical processes for molecules in external fields is dissociation [1]. New advances in ultrafast laser technologies [2] offer a whole set of powerful tools to control and explore molecular dissociation dynamics. In the past two decades, various strong-field dissociation mechanisms have been observed, such as bond softening [3], bond hardening [4], above threshold dissociation [5], zero photon dissociation [6,7], and rescattering dissociation [8]. In this paper we look into another less discussed mechanism for dissociation in the presence of an external field: tunneling dissociation. In this mechanism the nuclear wave packet tunnels through the light-induced barrier which binds the nuclei of the molecule.

When molecular ions are exposed to strong long-wavelength laser fields, the Coulomb barrier will be suppressed. Depending on laser intensities, some vibrational states can end up with energies higher than the barrier distorted by the laser fields, and hence these states will dissociate quickly. This phenomena is called overbarrier dissociation, in analogy to the overbarrier ionization of atoms and molecules in strong laser fields. Thachuk and Wardlaw [9] used classical trajectories to study the barrier-suppressed dissociation of HCl^+. This method was further developed by adding a hopping algorithm [10]. Later, Paci *et al.* [11] solved the two-channel time-dependent Schrödinger equation (TDSE) and analyzed the kinetic energy release of the proton in the barrier suppressed dissociation of H_2^+. Atabek *et al.* studied dynamical dissociation quenching and showed that by tuning the laser field intensities the molecular overbarrier dissociation may be suppressed or enhanced when the nuclear wave packet moves to the outer turning point [12–14]. Such dissociation control was also studied experimentally [15,16].

In a different scenario, the energies of vibrational states may remain lower than the laser-dressed Coulomb barrier. One may expect logically that tunneling dissociation will happen. Molecular tunneling dissociation has been discussed only in very few papers, partly because it is not possible to observe tunneling dissociation with current laser technologies. Wunderlich *et al.* [17,18] studied the dissociation of Ar_2^+ and explained that the nuclear wave packet may tunnel through the light-induced molecular potential. Chelkowski *et al.* [19] studied the tunneling dissociation of $dd\mu$, where the barrier is thin and the heavy nuclei may tunnel through within one femtosecond. For the simplest molecule H_2^+ and its isotopes, no evidence for tunneling dissociation has been reported until now.

In contrast, electron tunneling ionization [20] has been discussed extensively in literature and it is the basis of many strong-field phenomena observed such as high harmonic generation (HHG) [21,22] or multiple ionization by rescattering [23]. Generally, the mechanism for electron ionization in strong fields is characterized by the electronic Keldysh parameter [24] $\gamma_e = \sqrt{I_p/2U_{pe}}$ with I_p being the ionization potential and U_{pe} being the electronic ponderomotive energy. When $\gamma_e < 1$ ionization is said to occur through the tunneling mechanism. In this picture, the Coulomb barrier which binds the electron is deformed by the laser field for a relatively long time, compared to the time that the electron penetrates through the field-induced Coulomb barrier [25].

Inspired by this picture, we draft a similar definition to characterize the molecular dissociation and to classify it as tunneling, multiphoton, or overbarrier dissociation. We introduce the nuclear Keldysh parameter $\gamma_n = \sqrt{2D_p/U_{pn}}$ [11,19,26], where D_p is the dissociation potential and U_{pn} is the nuclear ponderomotive energy. Here $\gamma_n < 1$ refers to tunneling dissociation where the molecule dissociates after the nuclear wave packet goes through the light-induced potential.

The objective of this paper is to report observations of the tunneling dissociation of H_2^+ and characterize this process.

II. SIMULATION MODELS AND RESULTS

According to the electronic Keldysh parameter, for the hydrogen atom in a Ti:sapphire (800-nm) laser field, tunneling ionization occurs if the laser intensity is higher than

*fhe@sjtu.edu.cn

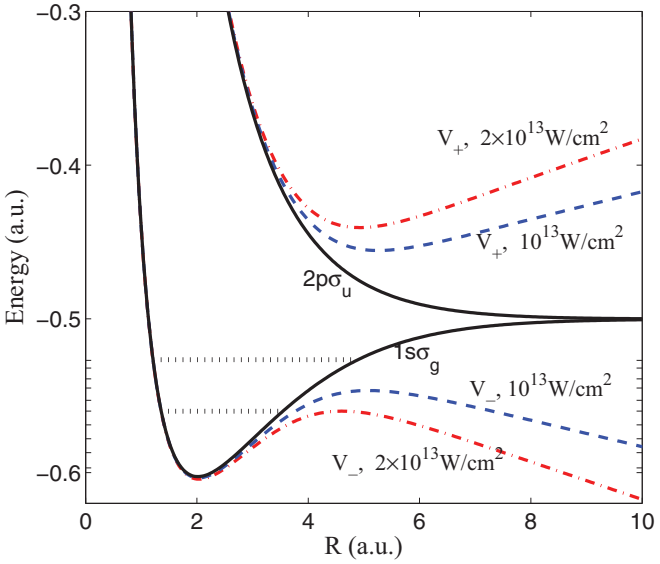

FIG. 1. (Color online) The potential curves of H_2^+ when the molecule is in the two lowest electronic states $1s\sigma_g$ and $2p\sigma_u$ in the field-free case (black solid lines), dressed by the field with intensities 10^{13} W/cm^2 (blue [gray] dashed lines) and 2×10^{13}W/cm^2 (red [gray] dash-dotted lines). The two horizontal dashed lines represent the energy levels of H_2^+ in the vibrational states $\nu = 4$ and $\nu = 9$.

10^{14} W/cm^2. Similarly, to make $\gamma_n < 1$ for H_2^+ in the vibrational ground state, the laser intensity has to be higher than 8×10^{16} W/cm^2 for 800 nm. However, such a high-intensity laser pulse will completely ionize H_2^+, preventing any dissociation of the molecule. In order to produce dissociation and avoid ionization, we choose a THz field with intensities $\sim10^{13}$ W/cm^2 which maintains the ionization level low and produces the desired $\gamma_n < 1$. Such a THz field could probably be produced due to the rapid advances in new light sources from laser-plasma interactions [27,28].

Tunneling dissociation only occurs if the time when the potential is distorted by the field is longer than the time the particle needs to cross the barrier. Therefore before doing quantum simulations, we use the WKB approximation to estimate the time that a nuclear wave packet takes to tunnel through the field-induced molecular barrier, as shown in Fig. 1, in which $V_\pm$ are the field-dressed adiabatic potential curves [29].

This so-called "tunneling time" [30] can be calculated as

$$T_I = \int_{R_{\rm enter}}^{R_{\rm exit}} \frac{dR}{|v(R)|}, \tag{1}$$

where

$$v(R) = \sqrt{2|E_\nu - V_-(R)|/\mu}. \tag{2}$$

Here, E_ν is the energy of the nuclear vibrational state with index ν. $R_{\rm enter}$ and $R_{\rm exit}$ are the roots of the equation

$$V_-(R) = E_\nu, \tag{3}$$

indicating the positions where the nuclear wave packets enter and leave the barrier.

These "tunneling times" are summarized in Table I, in which T_{I_1} and T_{I_2} correspond to laser intensities

TABLE I. Tunneling dissociation times (atomic units) of H_2^+, D_2^+, and T_2^+ in strong laser fields.

	H_2^+			D_2^+			T_2^+		
ν	E_ν	T_{I_1}	T_{I_2}	E_ν	T_{I_1}	T_{I_2}	E_ν	T_{I_1}	T_{I_2}
0	−0.597	1865	1341	−0.599	2570	1889	−0.600	3153	2328
1	−0.587	1662	1242	−0.592	2464	2199	−0.594	2968	2304
2	−0.578	1717	1310	−0.585	2288	1796	−0.588	2937	2147
3	−0.569	1457	1375	−0.578	2429	1853	−0.582	2811	2075
4	−0.561	1388	1384	−0.572	2180	1643	−0.577	2735	2115
5	−0.553	1451	0	−0.566	2088	1670	−0.572	2670	2012
6	−0.546	0	0	−0.560	1961	0	−0.567	2600	2136
7	−0.539	0	0	−0.555	2004	0	−0.562	2428	2317
8	−0.533	0	0	−0.549	2257	0	−0.558	2376	0
9	−0.527	0	0	−0.544	0	0	−0.553	2513	0

$I_1 = 10^{13}$ W/cm^2 and $I_2 = 2\times10^{13}$ W/cm^2, respectively. Zeros in the table mean that the vibrational energy levels are above the barrier, and hence the molecule will break via overbarrier dissociation [31].

When the field intensity is higher, more vibrational states participate in the overbarrier dissociation as expected. Comparing the molecules H_2^+, D_2^+ and T_2^+, we find that in heavier isotopes more vibrational states undergo tunneling dissociation. These times are much longer than the laser period of a Ti:sapphire laser, and therefore such a laser pulse cannot be used to observe the tunneling dissociation.

A complete three-dimensional (3D) ab initio simulation of the H_2^+ can be performed numerically [32,33] to study the tunneling dissociation, but the relevant time is very long, which makes simulations not practical. Further, for the proposed field parameters, ionization is not relevant and the important physics can be safely described using a simplified model. This model describes the evolution of the molecular wave packet in the ground and first excited electronic state of the molecule (atomic units are used unless otherwise stated)

$$i\frac{\partial}{\partial t}\begin{pmatrix}\chi_g(R,t)\\ \chi_u(R,t)\end{pmatrix} = \begin{pmatrix}T_R+V_g & V_{gu}\\ V_{gu} & T_R+V_u\end{pmatrix}\begin{pmatrix}\chi_g(R,t)\\ \chi_u(R,t)\end{pmatrix}, \tag{4}$$

where $T_R = -\frac{1}{2\mu}\frac{\partial^2}{\partial R^2}$ and μ is the reduced mass of the nuclei. χ_g and χ_u are the corresponding nuclear wave packets when the electron is in $1s\sigma_g$ and $2p\sigma_u$. The two lowest molecular potential curves V_g and V_u are shown in Fig. 1 by black solid lines, and V_{gu} is the dipole coupling between $1s\sigma_g$ and $2p\sigma_u$ states.

In following quantum simulations, we choose a laser field with wavelength of 0.1 mm (frequency 3 THz), and laser intensities 10^{13} W/cm^2 and 2×10^{13} W/cm^2. The electric field is expressed as

$$E = E_0\cos(\omega t)\sin^2(\pi t/\tau), \quad 0 < t < \tau, \tag{5}$$

where the pulse duration is $\tau = 4T$ and the laser period is $T = 13779$ a.u. For both laser intensities, the corresponding nuclear Keldysh parameter is smaller than 1, and the field period T is longer than the tunneling time shown in Table I. Therefore, tunneling dissociation is expected. In our simulations, the initial vibrational states are obtained by diagonalizing the Hamiltonian, and the Crank-Nicolson method is used to

propagate wave functions. Our simulations show the nuclear wave packet may extend to very large internuclear distances before nuclear rescattering happens, and therefore, we have to set a very large simulation box to include all the nuclear wave packets. The spatial and time grids are as small as $\Delta R = 0.01$ a.u. and $\Delta t = 0.1$ a.u. for obtaining converged simulation results. Two hundred thousand points are set in the R dimension, which covers the area $0 \sim 2000$ a.u.. Each simulation takes about 70 hours of computer processing time.

Atabek *et al.* [14] have show numerically that molecular rotation may change the dissociation probability if the driving laser field has a very long wavelength. The rotational period for H_2^+ in equilibrium internuclear distance is about several hundred femtoseconds and our driving laser pulse has duration more than 1 ps. Once the molecular ion has dissociated, the internuclear distance will increase quickly, and the elongated H_2^+ can be effectively aligned along the polarization axis of the driving THz field. Hence, we neglect the molecular rotation in our model. The dissociation probability may change quantitatively after considering the rotation and vibration simultaneously [14]; however, the reduced one-dimensional model is very good to explore qualitatively the tunneling dissociation mechanism.

To confirm that the ionization of H_2^+ can be neglected, we calculate the ionization probability with the one-dimensional fixed-nuclei model [34]. By scanning the internuclear distance, we find the largest ionization probability is less than 1% for the chosen laser parameters. The small ionization probability will deplete neither the bound vibrational states nor the dissociative states. Also, experimental techniques such as Cold Target Recoil Ion Momentum Spectroscopy (COTRIMS) [35] may easily distinguish ionization and dissociation channels. Therefore, we may neglect ionization when looking into the molecular dissociation for the given laser parameters in this paper. When the laser pulse is finished, we keep propagating the TDSE until all dynamics are converged. The dissociation probability is computed by integrating all nuclear wave packets distributed in the range $R > 20$ a.u.,

$$P_{\rm diss} = \int_{20}^{2000} dR[|\chi_g(R,t_f)|^2 + |\chi_u(R,t_f)|^2]. \qquad (6)$$

Figures 2(a), 2(b), and 2(c) show the final dissociation probabilities for molecules in different initial vibrational states when the field intensity is 10^{13} W/cm^2 (circles) and 2×10^{13} W/cm^2 (squares). Figure 2(d) shows the dissociation probability as a function of the field intensity when H_2^+ is initially in the vibrational state $\nu = 4$. Each curve in panels (a), (b), and (c) is divided in two different parts marked as black bold and light red (gray) lines. These two parts have two distinct slopes, indicating two different dissociation mechanisms: tunneling and overbarrier dissociation. For H_2^+, the inflexion points of these two dissociation mechanisms are found at the vibrational states $\nu = 6$ and $\nu = 5$ when laser intensities are 10^{13} W/cm^2 and 2×10^{13} W/cm^2, respectively. Isotopes D_2^+ and T_2^+ have similar behaviors although in flexion points occur at other vibrational states. These quantum simulation results are consistent with the results from the Wentzel–Kramers–Brillouin (WKB) approximation in Table I. When comparing the same vibrational states for different isotopic molecules,

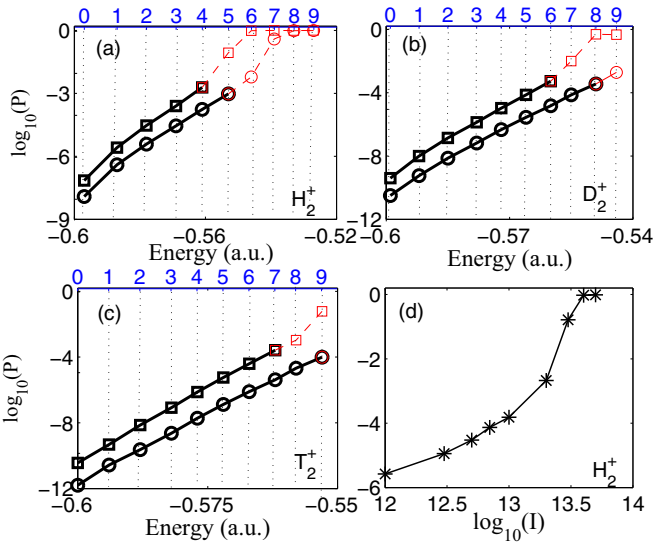

FIG. 2. (Color online) The dissociation probability P in logarithmic scale of (a) H_2^+, (b) D_2^+, and (c) T_2^+ initially in different vibrational states when the laser intensity is 10^{13} W/cm^2 (circles) and 2×10^{13} W/cm^2 (squares). The abscissas on tops of panels indicate the indices of nuclear vibrational levels. (d) The dissociation probability as a function of laser intensity for H_2^+ initially in the vibrational state $\nu = 4$.

lighter molecules have smaller dissociation potentials D_p and larger nuclear ponderomotive energies U_{pn}, leading to smaller γ_n. Hence, lighter molecules are easier to tunneling dissociate. This remark also works for heteronuclear hydrogen molecular ions, such as HD^+.

In Fig. 2(d), the dissociation probability increases very quickly as the laser intensity increases to 2×10^{13} W/cm^2, which is indeed the critical intensity where the transition between tunneling and overbarrier dissociation occurs according to the WKB estimation. In the upper-right corners of Figs. 2(a), 2(b), and 2(d), dissociation probabilities are saturated.

The molecular tunneling dissociation formula [19] cannot reproduce the quantum simulation results presented in Fig. 2, since the nuclear wave-packet distribution is very different from that of $dd\mu$, or some atomic bound states.

Tunneling ionization in many cases is followed by electron rescattering, which plays a central role in high harmonic generation [21,22] and double ionization [23]. Similarly, after the tunneling dissociation of H_2^+, two nuclei have the probability to rescatter each other once the electric field changes the direction. Figure 3(a) shows the nuclear wave-packet propagation in position space, i.e., $|\chi_g(R,t)|^2 + |\chi_u(R,t)|^2$. The laser intensity is 2×10^{13} W/cm^2, and the initial nuclear vibrational state of H_2^+ is $\nu = 3$. The nuclear quiver radius is about 125 a.u., which is very different from dynamical dissociation quenching (DDQ) [12–14], in which case nuclear wave packets vibrate within the range $1 < R < 10$ a.u.. The inset in Fig. 3(a) is an expanded view of the wave function for small internuclear distances. The inset clearly shows that the internuclear distance can be smaller than 1 a.u. at instants around $t = 600$, 800, and 1000 fs, which is a direct proof for nuclear rescattering.

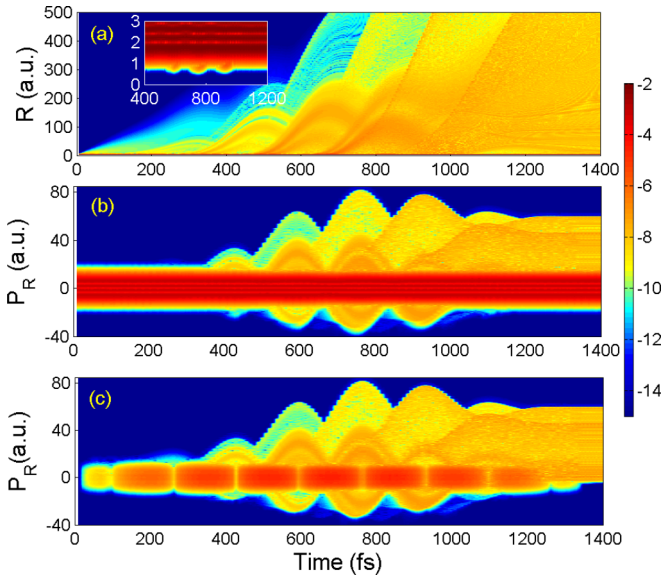

FIG. 3. (Color online) (a) H_2^+ nuclear wave-packet propagation in position representation. (b), (c) The propagation of $1s\sigma_g$ and $2p\sigma_u$ components of H_2^+ in momentum representation, respectively. The laser intensity is 2×10^{13} W/cm^2, and the initial vibrational state is $v = 3$. The inset in panel (a) is the zoom of panel (a) in the range of small internuclear distances. Logarithmic scales are used in all panels.

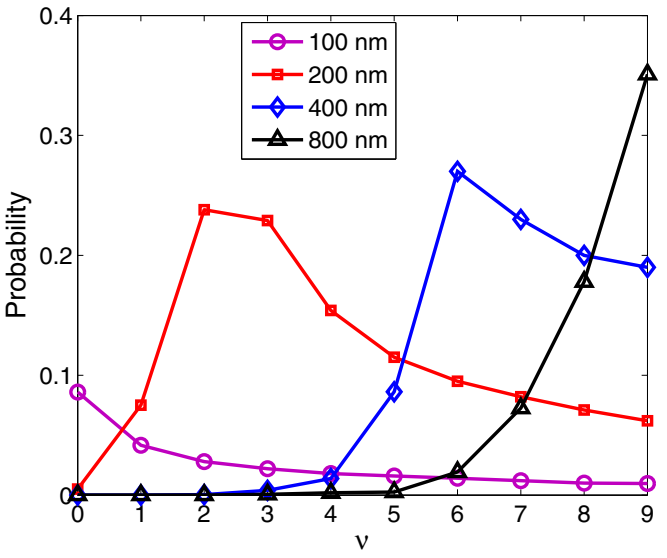

FIG. 4. (Color online) The dissociation probability of H_2^+ exposed to laser fields with wavelengths 100, 200, 400, and 800 nm. The laser intensity is 2×10^{13} W/cm^2 and each pulse comprises 15 optical cycles.

This rescattering can also be confirmed by the nuclear relative momentum distribution. We Fourier transform the nuclear wave packet into momentum representation and show in Figs. 3(b) and 3(c) the time-dependent wave packet in momentum representation $|\tilde{\chi}_g(p_R,t)|^2$ and $|\tilde{\chi}_u(p_R,t)|^2$, respectively. If the nuclear relative momentum is 0 initially, then the final nuclear momentum after tunneling dissociation is $A(t)/2$ [29] if no rescattering occurs, with $A(t)$ the vector potential at the time of tunneling dissociation. Figures 3(b) and 3(c) clearly show that some nuclear relative momenta are much larger than $\max(A(t)/2) = 26$ a.u., which can only be explained by the nuclear rescattering. Unlike in DDQ [12–14], where only the $1s\sigma_g$ component is involved, here both $1s\sigma_g$ and $2p\sigma_u$ components take part in nuclear rescattering. Except for the bound vibrational states, the nuclear wave packets propagating on both potential surfaces have very similar behaviors. In order to further support the rescattering explanation, we also solve the Newtonian equation [29] to confirm that the internuclear distance can be close to zero during the evolution (not shown).

Compared to tunneling dissociation, multiphoton dissociation shows a very different behavior. Figure 4 shows the dissociation probability of H_2^+ initially in different vibrational states, dressed by laser fields with wavelengths 100, 200, 400, and 800 nm. Laser intensities are 2×10^{13} W/cm^2, and each pulse comprises 15 optical cycles. For these wavelengths, the resonant one-photon transitions between $1s\sigma_g$ and $2p\sigma_u$ happen at different internuclear distances R_c, and dissociation probabilities depend on probability densities $|\chi_g(R_c)|^2$. For a longer wavelength, the peak of the dissociation probability shifts towards higher nuclear vibrational states. This is because higher vibrational states are spatially distributed around larger internuclear distances, enabling resonant transitions with smaller photon energies.

III. CONCLUSION

In conclusion, our simulations show strong evidences that H_2^+ and its isotopes can dissociate by tunneling in a long wavelength strong THz field. This is in contrast to short wavelengths which induce dissociation by multiphoton absorption. By looking at the dependence of the dissociation probability on the dissociation potential and the laser intensity, we are able to distinguish tunneling and overbarrier dissociation. After the tunneling dissociation of H_2^+, the molecular internuclear distance stretches to large values and the proton gains high kinetic energy, followed by nuclear rescattering once the laser electric field changes directions. The nuclear rescattering contributes to high momenta of the dissociating fragments, which does not occur in any other scenario. This process is the nuclear analogy to the well-known electron rescattering after tunneling ionization. With the fast development of new radiation sources, we expect that tunneling dissociation could be observed with the advent of the new bright THz sources in the near future.

ACKNOWLEDGMENT

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