Nuclear classical dynamics of H₂ in an intense laser field

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Abstract
In the first part of this paper, the different distinguishable pathways and regions of the single and sequential double ionization are determined and discussed. It is shown that there are two distinguishable pathways for the single ionization and four distinct pathways for the sequential double ionization. It is also shown that there are two and three different regions of space which are related to the single and double ionization, respectively. In the second part of the paper, the time-dependent Schrödinger and Newton equations are solved simultaneously for the electrons and the nuclei of H₂, respectively. The electron and nuclei dynamics are separated on the basis of the adiabatic approximation. The soft-core potential is used to model the electrostatic interaction between the electrons and the nuclei. A variety of wavelengths (390, 532 and 780 nm) and intensities (5 × 10¹⁴ and 5 × 10¹⁵ W cm⁻²) of the ultrashort intense laser pulses with a sinus second-order envelope function are used. The behaviour of the time-dependent classical nuclear dynamics in the absence and presence of the laser field is investigated and compared. In the absence of the laser field, there are three distinct sections for the nuclear dynamics on the electronic ground state energy curve. The bond hardening phenomenon does not appear in this classical nuclear dynamics simulation.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
Atoms and molecules exposed to intense laser pulses reveal a vast wealth of fascinating phenomena, for example single and double ionization [1], above-threshold ionization [2], charge resonance enhanced ionization [3], dissociative-ionization [4, 5], above threshold dissociation [6], bond softening and hardening [7–10] and high-order harmonic generation [11]. Scientific research regarding these phenomena resulted in a revolution in ultrashort laser pulses and molecular science with many broad applications such as the control of the molecular processes [12], generation of a few cycles of femtosecond and attosecond pulses, the emergence of the attophysics [13] and time-resolved imaging of molecular dynamics and reactions [14].

Our knowledge about the interaction of atoms and molecules with ultra-short intense laser pulses has proceeded like, essentially, all other fields of atoms and molecules from simple systems such as hydrogen atoms and hydrogen molecules to complex ones such as proteins. The first step in the chain of studying many-electron systems is the investigation of the simplest two-electron systems, i.e. helium atoms and H₂ diatomic molecules [15–17]. The response of many-electron atoms or molecules to the pulse of the laser field is often described by assuming that only one electron is active and responsible for the emission; this is called the single active electron (SAE) approximation. In this approximation, other electrons are assumed to contribute to the dynamics through a static screening potential. However, for a full description and to understand the behaviour of the two-electron systems, it is necessary to consider both electrons simultaneously without the SAE approximation. This work plays a central role in developing our understanding of the interaction of many-electron atoms and molecules with ultrashort intense laser fields [15–17]. For this purpose, we need to solve the time-dependent Schrödinger equation (TDSE) for the two-electron systems. This work is impossible with the current available computing power. Therefore, at the present time unavoidably in many research works, modelling of the interaction of two-electron systems with the laser pulse is accomplished by...
the so-called soft-core Coulomb potentials which makes the numerical solution of TDSE possible [18–22].

In this work, we consider the nuclei as classical particles. This model reduces the complexity of the problem and helps to show details of the dynamics of the electrons without the necessity that we get involved in complexities of the dissociative-ionization process [4, 5, 23–26]. In this research, the indistinguishability concept and the symmetry properties between two electrons will be demonstrated with some details. The main focus of attention in this paper is given to details of the classical nuclear dynamics and in a separate article details of the electron dynamics are represented [27].

The paper is organized as follows. In sections 2 and 3, details of the numerical solution of the TDSE and simulation box are described. In section 4, results of the simulations for the field-free case and also for different intensities and wavelengths are presented and discussed. Finally, the conclusion appears in section 4. We use the atomic units throughout this paper unless stated otherwise.

2. Numerical solution of the TDSE

In this section, we introduce details of the numerical solution and also the simulation box that we used for investigating the dynamics of the hydrogen molecule in the presence of a strong laser field. In a linearly polarized laser pulse with an intensity of up to $1 \times 10^{17}$ W cm$^{-2}$, most of the electron and nuclei dynamics occur in the direction of the laser field [21]. Therefore, we choose a one-dimensional model for the coordinates of both the electrons and nuclei. In what follows $R_1$ and $R_2$ indicate the nuclei positions, and $z_1$ and $z_2$ indicate the electron positions. Furthermore, $M$ and $m$ indicate the masses of the nuclei and electrons, respectively, and $e$ is the electron charge. The temporal evolution of the electronic parts of such a system is described by the TDSE on the basis of the adiabatic approximation, i.e. [21, 28]

$$\frac{\partial \psi(z_1, z_2, t; R_1(t), R_2(t))}{\partial t} = H_e(z_1, z_2, t; R_1(t), R_2(t))\psi(z_1, z_2, t; R_1(t), R_2(t)), \quad (1)$$

where the electronic Hamiltonian for this system, $H_e(z_1, z_2, t; R_1(t), R_2(t))$, is given by

$$H_e(z_1, z_2, t; R_1(t), R_2(t)) = -\frac{1}{2m_e} \left[ \frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial z_2^2} \right] + V_C(z_1, z_2, t; R_1(t), R_2(t)), \quad (2)$$

$$V_C(z_1, z_2, t; R_1(t), R_2(t)) = \sum_{i,a=1}^{2} \left( \frac{-Z_a}{\sqrt{(z_1 - R_a)^2 + a}} \right) + \frac{1}{\sqrt{(z_1 - z_2)^2 + b}} + \frac{1}{\sqrt{(R_1 - R_2)^2 + c}} + \frac{(z_1 + z_2)E_0 f(t) \cos(\omega t)}{2}, \quad (3)$$

respectively. As this equation shows, we use a soft-core potential to model the electrostatic interaction among the electrons and the nuclei by the screening parameters $a$, $b$ and $c$. We choose $a = b = 1.0$, $c = 0.03$ [21]. The ground state energy and the equilibrium internuclear distance of $H_2$ become $-1.39$ and $2.13$, respectively, for this choice of parameter (see figure 1).

The laser–molecule interaction is formulated in the dipole approximation in length gauge ($-e \mathbf{r} \cdot \mathbf{E}(t)$), where $E_0$ is the laser peak amplitude and $\omega = 2\pi \nu$ is its angular frequency. The envelope of the laser pulse, $f(t)$, is set as

$$f(t) = \sin^2 \left( \frac{t}{\tau_1} \right), \quad (4)$$

where $\tau_1$ is the time duration of the field irradiation set at $\tau_1 = 8$ cycles in this work. One cycle is equal to 1.30 fs (53.78 au) and 1.77 fs (73.36 au) for 390 and 532 nm, respectively. After the mentioned time, the simulation continues for eight more cycles in which there is no laser field as shown in figure 2 to follow the behaviour of the system after turning off the laser field. In this simulation, the time step is set to $\delta t = 0.02$. The differential operators in equation (2) are discretized by the 11-point difference formulae which have tenth-order accuracies [29]. To solve the above TDSE numerically, we adopted

![Figure 1](image1.png)

Figure 1. Calculated electronic ground state surface of the hydrogen molecule on the basis of a one-dimensional model for both electrons.

![Figure 2](image2.png)

Figure 2. The used laser electric field in this paper has a sinus second-order envelop function with eight optical cycles.
a general nonlinear coordinate transformation for electronic coordinates. For the spatial discretization, we have constructed a finite difference scheme with a nonuniform (adaptive) grid for $z_1$ and $z_2$ electronic coordinates, which are finest near the nuclei and coarsest at the border regions of the simulation box.

More details of our calculations are described in our previous reports [29, 30]. The absorber regions are introduced by using fourth-order optical potentials at the $z_1$ and $z_2$ boundaries in order to capture the photoelectrons and prevent the reflection of the outgoing wave packets at the borders of the grid. More details of our calculations are described in our previous work [30].

In this work, we separate the electron and nuclei dynamics on the basis of the adiabatic approximation [21, 28]. We consider the electron dynamics in the quantum approach, while the nuclei dynamics are investigated in the classical manner. So, the time-dependent Schrödinger and Newton equations are solved simultaneously for the electrons and the nuclei, respectively. The equations that govern the nuclear dynamics are as follows [21]:

$$
M R_1(t) = F_{12}(t) + F_{1c}(t) + F_L(t)
$$

$$
M R_2(t) = F_{21}(t) + F_{2c}(t) + F_L(t),
$$

where $F_L(t) = eE_0 f(t)\cos(w t)$ is the laser forces exerted on each nucleus and $F_{21}(t) = -F_{12}(t)$ is the internuclear repulsion

$$
F_{21}(t) = -F_{12}(t) = \frac{R_2(t) - R_1(t)}{(c+ | R_2(t) - R_1(t) |^2)^{3/2}}.
$$

$F_{nc}$ is the attractive forces between the electrons and nuclei where $e$ and $n$ are related to the electrons and nuclei, respectively:

$$
F_{nc}(t) = -\int \int \frac{[R_n(t) - z_1] | \Psi(z_1, z_2, t) |^2}{[a + [R_n(t) - z_1] |^2}] \, dz_1 \, dz_2

-\int \int \frac{[R_n(t) - z_2] | \Psi(z_1, z_2, t) |^2}{[a + [R_n(t) - z_2] |^2}] \, dz_1 \, dz_2.
$$

These Newtonian equations are solved by the Verlet algorithm [31].

3. Different pathways and regions of the single and sequential double ionization

In this section, we focus on different phenomena which might occur as a result of the interaction of the hydrogen molecule with the intense laser fields such as dissociation and a serious kind of ionization process. Due to the Pauli exclusion principle, the electronic wavefunction must always be antisymmetric. We assume an initial singlet two-electron state, so that the spatial part, $\psi(z_1, z_2, t; R_1(t), R_2(t))$, of the two-electron wavefunction is symmetric. As is schematically shown in figure 3, the simulation box is constituted by two degrees of freedom which are related to the movement of the electrons along polarization directions. One of the directions of the electrons adjoins with the horizontal axis ($z_1$) and the other with the vertical one ($z_2$). Both of them include negative and positive halves. The symmetry of the wavefunction in the box is identified by the diagonal line (X) that traces from the bottom-left corner to the top-right corner. This symmetry provides some opportunity for saving the necessary CPU time and memory in the simulation and also increases the rate of the calculations. So, during computation, we can just consider the top part of the simulation box with respect to the X line. According to indistinguishability, the behaviour of the bottom part of the box will be the same as the top part. The outer red regions surrounding the inner regions of the simulation box show the boundary absorption which lets absorption of the outgoing single- and double-ionization wavefunctions.

At the beginning of the simulation, the hydrogen molecule is placed at an initial internuclear distance in the ground electronic state with the nuclei at rest. Then, the density distribution of the electron clouds and also the position of the nuclei are affected by the radiation of the laser field which leads to dissociation, ionization and accomplishment phenomena. As long as the system is not ionized and dissociated, the population remains in the H$_2$ region of figure 3.

We now review some different kinds of electron emissions from the H$_2$ region. If due to the irradiation, only one of the two bounded electrons is affected, then that electron goes away from the nuclei and the other one rests under the Coulomb attractive forces. As a result of this process, the system goes out from the H$_2$ region and enters the neighbouring H$_2^+$ region. This process is called single ionization. The single ionization
can occur through four pathways which are shown by arrows 1–4 in figure 3. Because of the indistinguishability, there are only two distinct pathways for the single ionization that can be presented by arrows 1 and 2, or by arrows 3 and 4. The pathways that are shown by arrows 3 and 4 are completely equivalent to arrows 1 and 2, respectively. In pathway 1, electron 2 \((e_2)\) goes away from nuclei in the positive direction, while in pathway 2, electron 1 goes away in the negative direction which is in the opposite direction of electron 2. The distinguishable movement in pathways 1 and 2 is due to the symmetry breaking of the system by irradiation. Therefore, there are two distinguishable regions labelled I and II which are related to the \(\text{H}_2^+\) region. In the absence of the laser field, the initial symmetric wavefunction remains symmetric with respect to negative and positive halves. Beyond the \(\text{H}_2\) region, the force of the external field overcomes the Coulomb forces on the ionized electrons. Therefore, outside the \(\text{H}_2\) region, the movement of the ionized electrons is controlled mainly by the laser field. In the presence of the laser field after first ionization, it is expected that the next ionization occurs. In this condition, the distance of the non-ionized electron increases and as a result the system goes out of the \(\text{H}_2^+\) and \(\text{H}_2^+(\text{II})\) regions, which are related to the single ionization, and enters the neighbouring \(\text{H}_2^+(\text{I})\) regions. The pathways of the second ionization are represented in the top region with respect to the X line and by arrows 5–8 in figure 3. Therefore, there are four distinguishable pathways for the second ionization. This procedure leads to the sequential double ionization. Figure 3 shows three recognized different regions which are related to the double ionization, namely \(\text{H}_2^{+(\text{I})}\), \(\text{H}_2^{+(\text{II})}\) and \(\text{H}_2^{+(\text{III})}\). The distinction of the \(\text{H}_2^{+(\text{I})}\) and \(\text{H}_2^{+(\text{II})}\) regions, such as the \(\text{H}_2^{+(\text{I})}\) and \(\text{H}_2^{+(\text{II})}\) regions in figure 3, is due to the radiation of the linearly polarized laser field that leads to the symmetry break between the left and right of the wavefunction. The behaviour of the system in the third region of the second ionization, i.e. the \(\text{H}_2^{+(\text{III})}\) region, is completely different. Results in [27] (see figure 9) show a higher probability of finding the system in \(\text{H}_2^{+(\text{III})}\) regions than in regions \(\text{H}_2^{+(\text{I})}\) and \(\text{H}_2^{+(\text{II})}\). This is due to the tendency of the system to remain in a more stable region. When the system is in the \(\text{H}_2^{+(\text{III})}\) region, the two electrons emit from the nuclei in the opposite directions and as a result the system has the least feasible inter-electronic repulsion. In the \(\text{H}_2^{+(\text{I})}\) and \(\text{H}_2^{+(\text{II})}\) regions, both electrons are in the same positive or negative direction. In this situation, the repulsive force between the two electrons makes the system more unstable. Therefore, it is expected that the double ionization with opposite directions \(\text{H}_2^{+(\text{III})}\) is more probable than the double ionization with the same negative \((\text{H}_2^{+(\text{I})})\) or positive \((\text{H}_2^{+(\text{II})})\) directions. As shown in figure 3, the boundary absorption has been placed in the end of the regions of the single and double ionization which allows absorption of the outgoing wavefunction.

The indistinguishability of two electrons remains unchanged in the intense laser field but the ionization process occurs via various distinguishable pathways. There are two different pathways for the single ionization and four different pathways for the double ionization. In the double-ionization case, two electrons may go out from the right or left side of the simulation box. In the third pathway, the two electrons go out of the opposite sides.

4. Results and discussion

The electronic ground state of the hydrogen molecule is calculated by the imaginary time propagation method. The obtained potential energy curve is presented in figure 1. The electronic ground state energy is zero for the internuclear distance of 0.452 16 au. The minimum energy is \(-1.39\) au and the related equilibrium distance for the classical nuclear motion is 2.13 au.

First, we study the field-free behaviour of the system. Details of the size of the simulation box for the field-free calculation are as follows. The grid points for each \(z_1\) and \(z_2\) coordinates are 1110. The finest grid size value in an adaptive grid scheme is equal to 0.2 au for both \(z_1\) and \(z_2\) coordinates. The grids extend up to \(z_1 = \pm 114\) au. The size of the absorber regions equals \(\pm 14\) au. Therefore, the size of the simulation box equals 200 \(\times\) 200, regardless of the absorber regions. In the present laser field, different sized simulation boxes are used for the simulation box that is characterized.

In field-free simulations, at the initial time, the system is released at the different internuclear distances, the inner or outer turning points. The calculation shows three different sections on the electronic ground state energy curve. The first section is related to the internuclear distance smaller than 1.4 au (\(R_0 < 1.4\) au), the next section is related to the interval between 1.4 and 5 au (1.4 < \(R_0 < 5\) au) and the last section is for the internuclear distances which are greater than 5 au (\(R_0 > 5\) au). Since in the first section (\(R_0 < 1.4\) au) the nuclei are very close and the Coulomb repulsive force is so large, the system is unstable and the dissociation takes place easily. The smaller the internuclear distance, the faster the dissociation process. However, the reduction in the population of the electrons and the resultant ionization value is ignorable in this section. If the system is released in an internuclear distance belonging to the second section (1.4 < \(R_0 < 5\) au), which we call the potential well section, the ionization and dissociation do not occur, as shown in figure 4. By time evolution, the system just oscillates around the equilibrium internuclear distance. As the initial internuclear distance becomes closer to the equilibrium point, the period of the oscillation decreases and, as a result, the symmetry in the oscillation curve increases. At the equilibrium point, there is no oscillation. The antisymmetric which is observed in the oscillation cycle in the initial internuclear distances which are far away from the equilibrium point is due to the antisymmetric in the shape of the potential barrier walls. For example, the behaviour of \(R_0 = 1.9\) au is relatively symmetric about the equilibrium but the behaviour of 1.5 au is completely antisymmetric about the equilibrium point (2.13 au). Figure 4 shows that \(R_0 = 1.5\) and 3.9 au are the related inner and outer turning points, respectively. In the third section (\(R > 5\) au), the Coulomb force is very weak and the bounding between the nuclei is not very strong, so the dissociation does not occur unless the nuclei move to a greater internuclear distance at the initial time.
In the presence of the laser field, at first we discuss the effect of the size of the simulation box on the nuclear dynamics. The calculations show that in the higher intensity ($5 \times 10^{15}$ W cm$^{-2}$), the time-dependent internuclear distance for different sized simulation boxes is the same as $200 \times 200$. In the lower intensity ($5 \times 10^{14}$ W cm$^{-2}$), the results for the various sizes of the simulation box are shown in figure 5. This figure shows that during eight cycles of the laser pulse, there is a small difference in the internuclear distances for the various sizes. After eight cycles, the difference in these internuclear distances becomes considerable and the increase in the size of the simulation box does not result in the convergence of the time-dependent internuclear distance. We changed our explanation in the paper as below: we can explain these results as follows. In the higher intensity of the laser pulse ($5 \times 10^{15}$ W cm$^{-2}$), the increasing size of the simulation box does not affect the nuclear dynamics. At this intensity, two electrons become completely far from nuclei during a few cycles of the laser pulse and a dominant Coulomb explosion occurs between nuclei. Therefore, the increasing size of the simulation box does not affect the behaviour of the nuclear dynamics. On the other hand, at the lower intensity, the electrons do not move completely far from the nuclei. Therefore, both the Coulomb repulsion and the population of the electron about nuclei determine the time-dependent internuclear distance. Therefore, when the size of the simulation box increases, the remaining population of electrons around the nucleus in the simulation box before absorption by boundary absorption becomes slightly more and the magnitude of the Coulomb repulsion between the nucleus is decreased.

The behaviour of the system under the action of the laser irradiation is different from what is seen in the absence of the laser field. Figure 6 shows the time-dependent internuclear distance for three different wavelengths and two different intensities. In this figure, the size of the simulation box for the $5 \times 10^{15}$ W cm$^{-2}$ intensity is $200 \times 200$ and for the $5 \times 10^{14}$ W cm$^{-2}$ intensity is $300 \times 300$. In addition, figure 7 represents the time-dependent behaviour of the population (the residual norm in the simulation box that is equal to the total population of different regions in figure 3) in the simulation box for three different wavelengths and the two intensities of $5 \times 10^{14}$ and $5 \times 10^{15}$ W cm$^{-2}$. In this figure, the size of the simulation box for both intensities is $200 \times 200$. The reduction of population is due to the emission of the electrons from the absorption boundaries, shown in figure 3, that results in the single and double ionization. In a separate paper, we have shown details of the single and double ionization [27]. The results of figures 6 and 7 show, respectively, the magnitude of the internuclear distance (dissociation) and ionization for different sections and it is interesting to make a comparison with the results of the field-free case in figure 4. In the first panel in figures 6 and 7, i.e. $R_0 = 0.7$ au that belongs to the first section ($R_0 < 1.4$ au), the dissociation occurs, similar to what happens in the absence of the laser field. We also observe a notable decline in the norm of the system which means that the population of the electrons has left the computation box and ionization has occurred. The panels with $R_0 = 1.5, 2.13, 3.0$ and 3.9 au in figures 6 and 7 belong to the second section, i.e. (1.4 au $< R_0 < 5$ au), and in contrast to the field-free case both ionization and dissociation have occurred.

An interesting point in figure 6 is that the bond hardening phenomenon does not appear anywhere in these classical nuclear dynamics simulations. The bond hardening can occur when the laser field causes the nuclei to come closer to each other with respect to the field-free case. The meaning of the bond hardening in the quantum nuclear dynamics investigation, that was reported in the previous experimental and theoretical research [7–9], is vibrational trapping. In vibrational trapping, the molecular wave packet is trapped in a laser-induced potential well. In contrast to the intuitive expectations, increasing the laser intensity can lead to the temporary stabilization of the molecular bond. However, clear confirmation of bond hardening (or vibrational trapping) has remained elusive and might benefit from a fresh look [10].

In the last panel, with $R_0 = 5.0$ in figures 6 and 7, which is related to the third section ($R_0 > 5$ au), in contrast to the field free situation, both dissociation and ionization occur. In this section, the nuclei separate from each other slower in comparison with the second section, but the ionization rate is higher than that in the second section.
In all panels of figures 6 and 7, we can see that the electrons under the influence of the laser field move away from the nuclei, which leads to the Coulomb explosion between the nuclei. The Coulomb repulsion for the second section is stronger than that for the third section, which is due to the smaller initial internuclear distance in the second section when Coulomb expulsion is started.

Figure 6 shows that the speed of the dissociation increases with increasing wavelength or intensity of the laser field. This figure also shows that in the first section the wavelength is more effective than the intensity. In fact, for the longer wavelengths, the nuclei separate from each other more quickly since in this case, the system is irradiated for a longer time in each half cycle of the laser field without a change in the direction of the laser field. However, in the second section, the influence of the intensity overcomes the wavelength influence relatively. In fact, in the second section, the internuclear distance is closer to the equilibrium point, the more the speed of the nuclei separation is increased by the intensity.

Figure 7 shows that the population reduction starts with increasing wavelength and intensity. It should be mentioned that due to the increment of the stability of the system by getting closer to the initial equilibrium internuclear distance ($R_0 = 2.13$ au), the population reduction is decreased. This figure also represents that in the second section for the smaller wavelengths, the ionization appears before the beginning of

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**Figure 6.** The time-dependent internuclear distance for the three wavelengths and two different intensities and a comparison with the results of the field-free case in figure 4.
Figure 7. The time dependence of the population for the different initial internuclear distances for the three wavelengths and two different intensities.

the dissociation, which shows that the laser irradiation makes Coulomb explosion by forcing the electrons to move away from the nuclei.

5. Summary

In this work and [27], we tried to fundamentally pay attention to the subject of how two electrons behave and interact in a two-electron molecule in the simplest classical manner of nuclear dynamics. In the first part of this paper, the distinguishable pathways and regions of the single and sequential double ionization are determined and discussed. It is shown that the single ionization can occur through four pathways, but there are just two distinct pathways for the single ionization because of the indistinguishability of the electrons. This distinguishability of the two pathways is due to the symmetry break between the right and left coordinates, which is caused by the linearly polarized laser field. In the absence of the laser field, there are no such distinguishable pathways for electrons. The result leads to the appearance of two distinguishable regions for the \( \text{H}_2^+ \) region in a linearly polarized intense laser pulse. It is also shown that there are four distinct pathways for the ionization of the second electron. We showed that there are two different regions which are related to the single ionization and three different ones that are related to the double ionization. Among the regions of the second ionization, the \( \text{H}_2^{++} \) (III) region is more stable than the other two regions. In this region, the two electrons move away from the nuclei in opposite directions and as a result the system has
the least feasible inter-electronic repulsion. However, in the H2+(I) and H2+(II) regions, the two electrons move away in the same positive or negative direction.

In the second part of this paper, the time-dependent Schrödinger and Newton equations are solved simultaneously for the electrons and the nuclei of H2, respectively. These calculations show that there are three different sections on the electronic ground state energy curve in the absence of the laser field. In the first section (R0 < 1.4 au), the system is unstable and the dissociation takes place easily. However, the ionization value is ignorable in this section. In the potential well section (1.4 au < R0 < 5 au) ionization and dissociation do not occur. The system just oscillates around the equilibrium internuclear distance. As the initial internuclear distance becomes closer to the equilibrium point, the period of the oscillation decreases and, as a result, the symmetry in the oscillation curve increases.

At the equilibrium point, there is no oscillation. In the third section (R > 5 au), the dissociation does not occur unless the nuclei move to a greater internuclear distance at the initial time. In the presence of the laser field, in all three sections, the reduction of the population of the electrons appears in contrast to the field-free case. The speed of the dissociation increases with increasing wavelength or intensity of the laser field. In the first section, the wavelength is more effective than the intensity. In the second section, the influence of the intensity overcomes the wavelength influence. In the third section (R0 > 5 au), the nuclei move away from each other slower in comparison with that in the second section, but the ionization rate is higher than that in the second section. In the presence of the laser field, the time-dependent nuclear distance is independent of the size of the simulation box at the higher intensity (5 × 10^{15} W cm^−2), but at the lower intensity (5 × 10^{14} W cm^−2), the final magnitude of the nuclear distance depends on the size of the simulation box. Finally, the bond hardening phenomenon does not appear anywhere in these classical nuclear dynamics simulations.

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References

[1] Alnaser A S, Osipov T, Benis E P, Wech A, Cocke C L, Tong X M and Lin C D 2003 Phys. Rev. Lett. 91 163002
[2] Brabec T (ed) 2008 Strong Field Laser Physics (Springer Series in Optical Sciences) (Berlin: Springer)
[3] Zuo T and Bandrauk A D 1995 Phys. Rev. A 52 R2511
[4] Vafae M 2008 Phys. Rev. A 78 023410
[5] Leth H A, Madsen L B and Molmer K 2009 Phys. Rev. Lett. 103 183601
[6] Giusti-Suzor A, Mies F H, DiMauro L F, Charron E and Yang B 1995 J. Phys. B: At. Mol. Opt. Phys. 28 309
[7] Bandrauk A D and Sink M L 1981 J. Chem. Phys. 74 1110
[8] Frasinski L J, Posthumus J H, Plummeridge J, Codling K, Taday P F and Langley A J 1999 Phys. Rev. Lett. 83 3625
[9] Murgakvelidze M, He F, Niederhausen T, Litvinyuk I V and Thumm U 2009 Phys. Rev. A 79 033410
[10] Frasinski L J, Posthumus J H, Plummeridge J, Codling K, Taday P F and Langley A J 1999 Phys. Rev. Lett. 83 3625
[11] Alnaser A S, Osipov T, Benis E P, Wech A, Cocke C L, Tong X M and Lin C D 2003 Phys. Rev. Lett. 91 163002
[12] Kiessig M F et al 2006 Science 312 246
[13] Brabec T and Krausz F 2000 Rev. Mod. Phys. 72 545
[14] Bisgaard C Z et al 2009 Science 323 1464
[15] Haessler S et al 2010 Nat. Phys. 6 200
[16] McKeen J, Sayler A M, Gaire B, Johnson Nora G, Katanforoush A and Corkum P B 1994 Phys. Rev. A 49 2117
[17] Dehghiani E, Bandrauk A D and Kamga L Gmagm 2010 Phys. Rev. Lett. 81 061403
[18] Eberly J H 1990 Phys. Rev. A 42 5750
[19] Kulander K C, Mies F H and Schäfer K J 1996 Phys. Rev. A 53 2562
[20] Kitzner A, Grossmann F, Schmidt R and Rost J M 2010 Phys. Rev. A 81 020341
[21] Camiolo G, Castiglia G, Corso P P, Fiordilino E and Marangos J P 2009 Phys. Rev. A 79 063401
[22] Saugout S, Charron E and Cornaggia C 2008 Phys. Rev. A 77 023404
[23] Ergler T, Rudenko A, Feuerstein B, Zrost K, Schrøder C D, Chelkowski S, Bandrauk A D, Staudte A and Corkum P B 2007 Phys. Rev. A 76 013405
[24] Litvinyuk I V, Alnaser A S, Comtois D, Ray D, Hasan A T, Kiefeler J-C and Villeneuve D M 2008 New J. Phys. 10 083011
[25] Jin Y J, Tong X M and Toshima N 2010 Phys. Rev. A 81 013408
[26] Vafae M, Sami F and Shokri B 2010 arXiv:1012.4063v1
[27] Rigamonti A and Carretta P 2009 Structure of Matter: An Introductory Course with Problems and Solutions (Berlin: Springer)
[28] Vafee M, Sabzian H, Vafee Z and Katanforoush A 2005 arXiv:physics/0509072v4
[29] Vafae M and Sabzian H 2004 J. Phys. B: At. Mol. Opt. Phys. 37 4143
[30] Verlet L 1967 Phys. Rev. 159 98
[31] Verlet L 1967 Phys. Rev. 165 201

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