Single-photon induced symmetry breaking of the electron localization and photoelectron directional emission in the dissociative ionization of H$_2$

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Abstract

By numerically solving the non-Born–Oppenheimer time-dependent Schrödinger equation of H$_2$ exposed to an isolated EUV laser pulse, we demonstrate the photoionization associated with the $2s\sigma_g$ and $3p\sigma_u$ dissociative states of H$_2^+$. The two asymptotically degenerate pathways with opposite parities may interfere and end up with the same kinetic energy release, resulting in the asymmetric electron localization on two nuclei. Due to dipole selection rule, the emitted photoelectron has the opposite parity with the associated H$_2^+$, and thus is also on the coherent superposition of states with odd and even parities, leading to the asymmetric directional emission of the photoelectron. The asymmetry is fundamentally determined by the phase difference of the $2s\sigma_g$ and $3p\sigma_u$ dissociation channels.

1. Introduction

Molecular dissociation has been a fundamental process and hot topic for several decades with the advent of ultrashort laser technologies. During the dissociation, the valence electron may selectively choose one of the nuclei and thus the asymmetric electron localization is formed. The asymmetric localization may be built by the interference of two degenerated pathways with opposite parities [1]. Alternatively, the asymmetry can be understood in a quasiclassical way, in which the growing interatomic barrier blocks the electron hopping between different nuclei [2]. The control of electron localization during molecular dissociation has attracted great interests over the past two decades. As the simplest molecule, H$_2^+$ and its isotope molecules play an important role in the understanding of electron localization. Charron et al [3] predicted that phase-locked two-color pulses could be used to induce asymmetry in the angular distribution of the emitted fragments. Later, Ray et al [1] used two-color (800 and 400 nm) pulses achieved the electron localization of ion energies in the regions of bond softening, above-threshold dissociation, and rescattering dissociation. Roudnev et al [4] proposed that the use of carrier-envelope phase-locked few-cycle laser pulse to control the electron localization. Such a strategy was first performed and confirmed by Kling et al [5] and continued to be implemented in subsequent experiments [6–10]. To enhance the degree of asymmetry, He et al [2] decoupled the excitation and steering using the attosecond pulse and the infrared pulse consequently, enhancing the electron localization. Sansone et al [11] implemented this strategy in later experiment and demonstrated the feasibility. He et al [12] also proposed that the use of an attosecond pulse train and a time-delayed near-infrared laser pulse to control the electron localization, which had been confirmed in the experiment [13]. Wu et al [14] used a single circularly polarized multicycle laser pulse to control the electron localization. Gong et al [15] used the orthogonally polarized two-color laser pulses realized the two-dimensional directional proton emission. Jia et al [16] achieved an extremely high degree of electron localization by using an ultraviolet pulse plus a THz pulse. In addition to the above control schemes, some
other strategies for controlling electron localization are also realized, such as half-cycle pulse train [17], phase-controlled elliptically polarized two-color laser pulses [18], subcycle waveform shaping by synthesizing coherent multicycle mid-infrared pulses of different wavelengths [19, 20], carrier-envelope phase-controlled multicycle laser pulse [21], phase-stabilized few-cycle mid-infrared laser pulse plus low-frequency field [22], plasmonic-enhanced laser field or spatially inhomogeneous near field [23, 24], and carrier-envelope phase-locked ultrashort chirped pulse [25].

The above control schemes for electron localization only consider the coupling between the two lowest electronic states of H$_2^+$, namely the ground state 1σ$_g$ and the first excited state 2σ$_g$. In many cases, the highly excited states may also involve the dissociation dynamics. McKenna et al [26] used advanced experimental and theoretical techniques revealed that highly excited states contribute significantly to the observation of high-order above-threshold dissociation. Dehmer et al [27] measured the ionic angular distributions of 2pσ$_g$, 2pπ$_g$, 2sσ$_g$ generated by the ionization of H$_2$ at photon energy of 40.8 eV and the branching ratio between the degenerate channels. At the same photon energy, Wu et al [28] measured the kinetic energy distributions of excited hydrogen atoms produced in the dissociative photoionization excitation of H$_2^+$, and determined the relative partial cross sections for direct dissociative photoionization excitation through the 2pπ$_g$ and 2sσ$_g$ states. Hikosaka et al [29] measured the correlation diagram between the kinetic energies of electrons and the energies of H$^+$ and the molecular-frame photoelectron angular distributions for ionization of H$_2$ to the 2pσ$_g$, 2pπ$_g$, and 2sσ$_g$ states of H$_2^+$. Chung et al [30] measured the absolute cross sections for the production of H$^+$ and H$_2^+$ from the dissociative ionization of H$_2$ at 18.076–124 eV, in which the 2pσ$_g$ and 2sσ$_g$ ionic states are fully accessible. To et al systematically measured the kinetic energy distributions of protons and deuterons produced by dissociative photoionization of H$_2$ and D$_2$ for photon energies of 25–45 eV [31, 32], and the molecular frame photoelectron angular distributions for the 2pπ$_g$ and 2sσ$_g$ ionic states of H$_2^+$ in the 44–76 eV photon energy range [33]. Jelovina et al [34] theoretically investigated the nuclear wave packet dynamics triggered by frequency-chirped ultrashort pulses in the excited states 2pσ$_g$ and 3pσ$_g$ of H$_2^+$.

In addition, since the high excited-state energy levels of H$_2^+$ are close in energy and different in symmetry, the coherent superposition of multiple dissociation channels is expected to break the symmetry of electron distribution on the nucleus. He [35] used orthogonally polarized two-color laser pulses to control electron localization in π orbitals. Wang et al [36] proposed a scheme to control the electron localization during the dissociation of H$_2^+$ along the highly excited states 2sσ$_g$ and 3pσ$_u$. Jia et al [37] used ultrashort ultraviolet laser pulses to excite electrons, and then used a direct current electric field to steer the motion of electrons in the lowest three excited states to control the electron localization.

Electron localization experiments are usually using the target H$_2$ instead of H$_2^+$, which requires considering two-electron correlations in theoretical calculations. In the above references, the two-electron correlation is neglected. Martín et al [38] have shown that the photoelectron emission symmetry can be broken if intermediate doubly excited states were populated and later decayed into 2pσ$_g$ and 1σ$_g$ states. Subsequently, they comprehensively investigated the photoelectron asymmetric emission caused by the participation of doubly excited states in the dissociative single ionization of H$_2$ under various laser parameters [39–42], and recently used an attosecond XUV pump/IR probe scheme to control the photoelectron asymmetric emission [43]. In their theoretical approach, the initial and final states are described in the framework of the Born–Oppenheimer approximation. In addition, recent studies showed that the two-electron correlation may modify the electron localization. Serov and Kheifets [44] predicted that after single ionization of H$_2$, the Coulomb interaction between the freed electron and the vibrating H$_2^+$ may pump H$_2^+$ from the 1σ$_g$ state to the 2pσ$_g$ state, making the bound electron preferentially locate on the nucleus moving oppositely to the photoelectron. Later, Waitz et al [45] and Heck et al [46] experimentally observed this asymmetric distribution and confirmed such dynamics. Wang et al [47] used the reduced-dimensionality numerical model to simulate such a process and the simulation results can quantitatively explain the experimental measurement, ensuring the feasibility of such a reduced-dimensionality numerical model. Recently, Martín et al [48] unraveled the role of electron–electron correlation in D$_2$ photoionization by mapping the dissociation of a highly excited D$_2^+$ molecule by combining state-of-the-art light sources and advanced detection techniques.

In this paper, we study the photoionization of H$_2$ and the subsequent dissociation of H$_2^+$, The theoretical scheme is shown in figure 1. An isolated EUV pulse singly ionizes H$_2$, and meanwhile excites H$_2^+$ to highly excited states such as 2sσ$_g$ and 3pσ$_u$ who have degenerate dissociation limits. The hybrid and interference of different dissociation pathways give rise to the asymmetric electron localization on the two nuclei. Due to the entanglement between H$_2^+$ and the freed electron, the photoelectron also presents asymmetric emission from the viewpoint of bound electrons. The phase difference between different dissociation pathways, which determines the electron localization, depends on the nuclear kinetic energy.
The rest of the paper is organized as follows. In section 2, we introduce the details of our simulation model. Then we show the numerical results in section 3. Finally, we give a summary in section 4.

2. Numerical models

For our numerical simulations, we have used the reduced dimensionality model (the electronic and nuclear motions are confined along the laser polarization direction) of H\(_2\) interacting with a linearly polarized pulse. The dynamics of H\(_2\) in strong laser fields is governed by the time dependent Schrödinger equation (TDSE) (atomic units, \(e = m = \hbar = 1\), are used unless indicated otherwise)

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \Psi(R, x_1, x_2; t) = [T + V(R, x_1, x_2)]\Psi(R, x_1, x_2; t),
\]

with the kinetic energy operator

\[
T = \frac{p_R^2}{2\mu} + \frac{[p_1 + A(t)]^2}{2} + \frac{[p_2 + A(t)]^2}{2}
\]

and the Coulomb potential

\[
V(R, x_1, x_2) = \frac{1}{R} + \frac{1}{\sqrt{(x_1 - x_2)^2 + \alpha(R)}} - \sum_{s=\pm 1} \sum_{i=1,2} \frac{1}{\sqrt{(x_i + sR/2)^2 + \frac{\alpha(R)}{2}}} + \frac{\beta(R)}{R} - \frac{\beta(R)}{2}.
\]

Here, \(\mu = 918\) is the reduced nuclear mass, and \(A(t)\) is the laser vector potential. \(p_R, p_1,\) and \(p_2\) are the relative nuclear momentum operator, and the momentum operators for two electrons. \(\alpha(R)\) and \(\beta(R)\) are the soft-core parameters used to obtain accurate potential energy curves, and their values are shown in figure 2 of reference [49]. The related Born–Oppenheimer potential curves given by this model are shown in figure 1. Though this model is hard to accurately describe the photoelectron momentum distribution, it is good enough to qualitatively grasp the electron–electron as well as electron–nuclei correlation [47, 50, 51]. Besides the dissociative ionization, this model has been used to deal with the double ionization of H\(_2\) [52, 53], high harmonic generation [54] and above-threshold dissociation [55]. In simulations, the spatial grids are \(\Delta x_1 = \Delta x_2 = 0.3\) a.u. and \(\Delta R = 0.02\) a.u., and the time step is \(\Delta t = 0.1\) a.u. Simulation convergence has been tested by using smaller time-spatial grids. The simulation box along \(x_1–x_2–R\) are sampled by the grids \(10,000 \times 160 \times 1600\). The procedure for the solution of equation (1) is provided in references [47, 49]. In simulations, we treat \(x_1\) as the electron to be ionized, and \(x_2\) as the bound one since \(x_2\) has a relatively small range.

The vector potential of a linearly polarized laser field is written as

\[
A(t) = A_0 \sin(\omega t)\sin^2\left(\frac{\pi t}{\tau}\right),
\]

where \(A_0, \omega,\) and \(\tau\) are the amplitude, frequency, and pulse width of the EUV pulse, respectively. The laser intensity is fixed at \(5 \times 10^{13}\) W cm\(^{-2}\) in this paper. The intensity is not a sensitive parameter since it is a one-photon process, and thus in the future experiment a weaker laser pulse may be implemented to demonstrate the scenario discussed in this paper. In simulations, we keep propagating the wave function
until the internuclear distance of dissociated $\text{H}_2^+$ along the $2s\sigma_g$ and $3p\sigma_u$ states are greater than 20 a.u., where the potential energy curves of the two states are degenerate. The electron–nuclei joint energy spectrum (JES) can be obtained by picking up dissociated wave-packets and Fourier transforming them into momentum space, i.e.

$$N(E_N, E_e) = \int \left| \tilde{\Psi}(p_1, x_2, p_R; t_{\text{end}}) \right|^2 p_1 p_R \, dx_2,$$

where $\tilde{\Psi}(p_1, x_2, p_R; t_{\text{end}})$ is the dissociative ionized wave-packet in the representation $p_1 - x_2 - p_R$ at the end of the simulation, $E_e = p_1^2/2$ and $E_N = p_R^2/2\mu$ represent the photoelectron energy and the sum kinetic energy of two nuclei. In all our simulations, $t_{\text{end}} = 800$ a.u.

The eigenstate of $\text{H}_2$ has well defined parity, which contribute to symmetric distributions. To break such a symmetry, at least two dissociative ionization channels ending with the same kinetic energy release (KER) and electron momentum must be ensured. The single-photon ionization of $\text{H}_2$ in the ground state gives a final eigenstate with odd parity. In this study, as indicated in figure 1, the dissociative ionization state can be expressed as

$$|\Psi\rangle = C_1 |2s\sigma_g\rangle \otimes |\epsilon_g\rangle + C_2 |3p\sigma_u\rangle \otimes |\epsilon_u\rangle,$$

where $|\epsilon_g/u\rangle$ denotes the states of the freed electron of energy $\epsilon$ and parity $g/u$. One may expect such a superposition states lead to the asymmetric distribution. We may point out that such asymmetry can not be achieved if one starts from any electronic eigenstate of $\text{H}_2^+$ instead of $\text{H}_2$. To describe the asymmetry quantitatively, we first divide the final dissociative ionization wave function $\Psi$ into the four parts belonging to the different spatial regions in the $x_1 - x_2$ space, as shown in figure 2, and then define the asymmetry parameter as

$$\delta_b = \frac{P_D - P_C}{P_D + P_C},$$

where $P_D$ and $P_C$ represent the probabilities computed from the wave function $\Psi_D$ and $\Psi_C$, respectively. In the above definition, we only concern the photoelectron emitting along the $-x$ axis. The asymmetric parameter of ionized electrons can be expressed as

$$\delta_f = \frac{P_A - P_C}{P_A + P_C},$$

where $P_A$ represents the probability computed from the wave function $\Psi_A$. It can be proved that $\delta_b = \delta_f$, since $\Psi_A(x_1, x_2, R) = \Psi_D(x_2, x_1, R) = \Psi_C(x_1, x_2, R)$ and $P_A = P_D$ for spin singlets. Such relationship is certainly ensured by our numerical simulations. In this paper, we only present the asymmetry parameter $\delta_b$.

To explore how the asymmetry parameter is dynamically formed, we investigate $\delta_b$ as a function of the freed electron energy and KER,

$$\delta_b(E_N, E_e) = \frac{N_D(E_N, E_e) - N_C(E_N, E_e)}{N_D(E_N, E_e) + N_C(E_N, E_e)},$$

Figure 2. Schematic diagram of the four spatial regions in $x_1 - x_2$ space used to calculate the asymmetry parameters.
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where \( N_C(E_N, E_e) = \int_{x_{\text{min}}}^{0} \frac{|\langle \Psi(x_1, x_2, R; t_{\text{end}}) | p | \Psi \rangle|^2}{|p| |\Psi\rangle} \, dx_2 \), and \( N_D(E_N, E_e) = \int_{x_{\text{max}}}^{x_{\text{max}}} \frac{|\langle \tilde{\Psi}(x_1, x_2, R; t_{\text{end}}) | p | \tilde{\Psi} \rangle|^2}{|p| |\tilde{\Psi}\rangle} \, dx_2 \). In later calculations, we pick up the dissociative ionized wave packet in the space \( R > 15 \) and \( x_1 + R/2 + 10 < 0 \) to calculate the asymmetry.

3. Simulation results

In the simulations, we used linearly polarized light with photon energies in the 40–57 eV range to ionize \( \text{H}_2 \). The laser pulse width is \( \tau = 60 T \), where \( T \) is the optical period of the laser field. In this range of photon energies, two typical pathways may occur. In the first case, one electron may carry all the excess energy, and \( \text{H}_2^+ \) in the 1\( \sigma_g \) state is formed. In the second case, one electron is stimulated with enough energies and freed, and the remaining ion is excited, for example, forming the \( \text{H}_2^+ \) in the 2\( \sigma_u \), 2\( \sigma_g \), 3\( \sigma_u \) and even higher excited states. In this paper, we focus on the excitation to 2\( \sigma_g \) and 3\( \sigma_u \) states, which have close potential curves and the same dissociation limit. As described before, the 2\( \sigma_g \) and 3\( \sigma_u \) states cannot be reached simultaneously by absorbing single photon if one starts from \( \text{H}_2^+ \) instead of \( \text{H}_2 \) due to the parity selection rule. However, for the \( (\text{H}_2^+, \text{e}^-) \) system, either \((u, g)\) and \((g, u)\) parity are allowed.

Figure 3 shows the snapshot of wave-packet distribution in the \( x_1 - R \) space, i.e., \( W(x_1, R; t_{\text{end}}) = \int |\Psi(x_1, x_2, R; t_{\text{end}})|^2 \, dx_2 \). The part marked by a red dashed rectangle corresponds to forming a freed electron and bound \( \text{H}_2^+ \), which is not of interest in this paper. The white dotted rectangle and pink dash-dotted oval correspond to the second case, producing a freed electron and dissociative \( \text{H}_2^+ \). Compared to the dissociation along the 2\( \sigma_g \) state, more energies deposit into \( \text{H}_2^+ \) if it is in a higher excited state, and thus the associated electron has smaller energy. Therefore, one can distinguish dissociative channels by selecting the electron in different energy ranges. For example, the part marked by a white dotted rectangle corresponds to producing \( \text{H}_2^+ \) in the 2\( \sigma_u \) state, and the wave-packet in the pink dash-dotted oval indicates \( \text{H}_2^+ \) in the 2\( \sigma_g \) or 3\( \sigma_u \) or even higher excited states.

Figures 4(a) and (b) show the JES corresponding to the wave function in the white dotted rectangle and pink dash-dotted oval in figure 3. We assume \( \text{H}_2 \) is aligned along the horizontal \( x \) axis. Figure 4(a) is for \( x_1 < 0, x_2 < 0 \), corresponding the dissociative ionization events \( \Psi_c \) in figure 2. Figure 4(b) corresponds to \( x_1 < 0, x_2 > 0 \), representing that the bound electron locates in the right nucleus. The two diagonal structures follow the curve \( E_N + E_e = E_{\text{c}} = E_{\text{DP}(n=1)} \). In this calculation, the photon energy is set to be \( E_\gamma = 54.4 \) eV, and \( E_{\text{DP}(n)} \) is the dissociative ionization potential for the \( p + \text{H}(n) \) channel. \( E_{\text{DP}(n=1)} = 17.4 \) eV is for the 2\( \sigma_g \) state, and \( E_{\text{DP}(n=2)} = 26.4 \) eV is for the 2\( \sigma_g \) and 3\( \sigma_u \) dissociation channels [48]. The energy conservation forces the JES along two diagonal lines in figures 4(a) and (b). These data present a similar structure to the experimental results and theoretical results in reference [48]. In addition, it can also be seen from figures 4(a) and (b) that the signals distributed along \( n = 1 \) are almost the same. This is attributed to the fact that only one dissociation channel contribute to the corresponding KER [39, 56–59]. However, the signals distributed along the \( n = 2 \) line in figures 4(a) and (b) are clearly

![Figure 3](image-url)
Figure 4. (a) and (b) The electron–nuclei JES. (c) The asymmetry parameter $\delta_b$ as a function of the nuclear energy $E_N$ and electron energy $E_e$. The dotted lines represent the energy conservation corresponding to total kinetic energies of 37 eV for $n = 1$ and 28 eV for $n = 2$. The spatial ranges of the two electrons are $x_1 = 1500$ a.u. and $x_2 = 24$ a.u., respectively. The laser parameters are the same as those used in figure 3.

different, due to the mixture of the 2$s\sigma_g$ and 3$p\sigma_u$ dissociation channels ending up with the same KER. Figure 4(c) shows the asymmetry parameter $\delta_b$ of bound electrons as a function of the nuclear energy $E_N$ and photoelectron energy $E_e$. For $n = 2$, when the energy carried by the free electrons is 6.6–11.2 eV, the bound electron prefers to locate in the right nucleus. When the energy carried by freed electrons is 11.2–14.5 eV, the bound electrons are mostly localized on the left nucleus. Accordingly, by picking the photoelectron in a certain energy range, the selective location of the bound electron in $H^+_2$ is achieved. Such preference is the manifestation of the entanglement between the remaining $H^+_2$ and free electron. Schöffler et al achieved ultrafast probing of core hole localization by experimentally measuring K-shell photoionization of $N_2$. They found that the intermediate core hole state is entangled with the Auger electron and the photoelectron [60, 61].

In principle, two electrons interact with each other during the whole process, which, however, does not mean the Coulomb repulsion between the two electrons significantly modifies the electron localization. This statement is confirmed by using a Yukawa potential as the electron–electron repulsion in our numerical model. Namely, we replace the electron–electron repulsion potential by

$$\frac{1}{\sqrt{(x_1-x_2)^2+\alpha(R)}}e^{-\frac{(x_1-x_2)^2}{\sigma^2}}$$

in equation (3). By changing $\sigma$ from 10 to 50 gradually, the asymmetry parameters keep unchanged. The conclusion is different from the conclusions in [44–47], where the photoelectron energy is about 2 eV and thus the photoelectron may interact with another bound electron in a relatively long time. In this paper, the photoelectron energy is around 20 eV so that it quickly flies away and the effect of electron–electron repulsion on the final state can be neglected. Furthermore, here we emphasize that when the Coulomb potential is replaced by the Yukawa potential, part of the doubly excited states are lost. However, for the photon energy used in this paper, only few doubly excited states are populated and we focus on the dissociation along the 2$s\sigma_g$ and 3$p\sigma_u$ states. Thus, the main physical results shown in this paper do not change noticeably.

Analytically, electron localization depends on the relative amplitude and relative phase of the two states. The former determines the quantity of the asymmetry parameter, and the latter governs the sign of the asymmetry parameter. While the TDSE simulation automatically comprises the phase term, a classical calculation may intuitively tell how the phase is accumulated during the dissociation. Here, we calculate the phase for nuclear wave packet propagating along the 2$s\sigma_g$ and 3$p\sigma_u$ potential energy curves in a classical manner [14]. Replacing the nuclear wave packet by a classical mass point, the movement of the mass point can be obtained by solving the Newtonian equation. Alternatively, the instantaneous nuclear momentum $p_{2s\sigma_g}(R)$ or $3p\sigma_u(R)$ can be calculated according to the energy conservation. The ultimate KER is determined by the staring internuclear distance $R_{i,g/u}$ where the mass point start. The phases are expressed as

$$\varphi_{2s\sigma_g}(E_N) = -E_{0,g}(t_f-t_0) + \int_{R_{i,g}}^{R_f} p_{2s\sigma_g}(R)dR,$$

$$\varphi_{3p\sigma_u}(E_N) = -E_{0,u}(t_f-t_0) + \int_{R_{i,u}}^{R_f} p_{3p\sigma_u}(R)dR.$$
Figure 5. The asymmetry parameter $\delta_b$ as a function of the nuclear energy $E_N$. The blue solid line is the result of the TDSE simulation. The red dashed line is obtained based on the classical model. The laser parameters are the same as those used in figure 3.

Figure 6. The asymmetry parameter $\delta_b$ as a function of the electron energy $E_e$ and photon energy. The laser intensity is $5 \times 10^{13}$ W cm$^{-2}$.

Here $t_0$ is the ionization time of H$_2$, and $t_f$ is the time when the internuclear distance is so large that energies of $2\sigma_g(R)$ and $3\sigma_u(R)$ potential curves are degenerate. We assume that just after the ionization of H$_2$, the nuclei already carry the kinetic energy $E_{0,\sigma_g}$, thus $E_{0,\sigma_g} = V_g/R_{g,\sigma_g} + E_{0,\sigma_g}$. The asymmetry parameter is proportional to $\cos(\varphi_{2\sigma_g}(E_N) - \varphi_{3\sigma_u}(E_N))$. In order to make the classical calculation fit with TDSE simulation, we set $E_{0,\sigma_g} = 0.1$ a.u. and $E_{0,\sigma_u} = 0.05$ a.u. Figure 5 shows the asymmetry parameter $\delta_b$ as a function of the nuclear energy $E_N$ obtained from the TDSE simulation. For comparison, the $\cos(\varphi_{2\sigma_g}(E_N) - \varphi_{3\sigma_u}(E_N))$ line is presented by the red-dashed line.

As shown by equation (10), the phase difference between the $2\sigma_g$ and $3\sigma_u$ states depends on the KER. In the dissociative ionization, the photon energy is shared between the photoelectron and nuclei, and thus the electron localization in H$_2^+$ should depend on the photoelectron energy though the Coulomb interaction between H$_2^+$ and the freed electron is negligible in this study. In simulations, we scan the photon energy from 40 eV to 57 eV, and show the asymmetry parameter $\delta_b$ as a function of the photon energy and electron energy $E_e$ in figure 6. Within the strips with slope 1 in figure 6, the KERs are actually the same, and so do the asymmetry parameters.

4. Conclusions

In conclusion, we have studied the asymmetric electron localization and asymmetric electron emission in the dissociative ionization of H$_2$ driven by an isolated EUV pulse. In the study, the photon energy is large enough to kick off one electron and simultaneously excite H$_2^+$ to the $2\sigma_g$ and $3\sigma_u$ states. Either the freed electron or the dissociative H$_2^+$ is on the superimposed states with odd and even parities. The mixture of the states with opposite parities leads to the asymmetric electron localization on the two nuclei and the asymmetric photoelectron emission. Due to the parity conservation of the whole system, the asymmetries of the freed electron and the bound electron are the same. This entangled system works as another version...
of Einstein–Podolsky–Rosen–Bohm paradox, i.e., by measuring the preferential emission direction of the freed electron, one may immediately acquire the localization of the bound electron on the two nuclei, regardless of how far the freed electron and the dissociative $\text{H}_2^+$ are separated [49].

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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