A quantum mechanical study of dissociative He + H₂ collisions

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Abstract

Accurate quantum mechanical calculations are made for a dissociative He + H₂ collision on a realistic potential energy surface by using the discrete-variable-representation (DVR) method of Sakimoto and Onda (J. Chem. Phys. 100 (1994) 1171). The molecular orientation (angle γ) relative to the intermolecular (He–H₂) axis is frozen in the calculation, and the molecular-orientation dependence of the dissociation is investigated by changing the angle as γ = 0 (collinear), π/4, and π/2 (T-shape). It is found that the dissociation probability is strongly dependent on the molecular orientation, and the molecule dissociates more frequently in the T-shape configuration rather than in the collinear one. Furthermore, the dissociation probabilities are compared with the results obtained by the standard close coupling (CC) method for the T-shape configuration (Nobusada et al., Chem. Phys. Letters 233 (1995) 399). The DVR method can provide accurate dissociation probabilities even in the case that convergence has not been fully achieved in the previous CC study.

1. Introduction

Collision induced dissociation (CID) is an important process in non-equilibrium gases [1], in shockwave phenomena [2–4], or in UV-absorbing gases [5]. To investigate their gas dynamics, the rate constants of CID must be given for molecules in various vibrational and rotational states. Since accurate quantum mechanical 3D calculations are quite difficult for the CID process, a quasiclassical trajectory (CT) method is usually invoked to obtain the rate constants [2,6]. The CT calculation may provide reliable results for the data needed. However, it does not mean that the CT method provides a full understanding of the dissociation mechanism. Also to assess its validity, the CT result should be compared with the quantum mechanical one. In addition, because of the difficulty in the description of the double continuum of scattering and dissociative states, it has not yet been well resolved how one can obtain the S-matrix elements for the CID process in quantum mechanical calculations [7–20]. For these reasons, it is highly desirable to promote a quantum mechanical study of CID.

Most of the previous quantum mechanical studies of CID have assumed a collinear collision [7–16,19,20]. Other collision configurations have been rarely considered [17,18]. However, unlike in the low-energy rearrangement reaction in which a transition state plays a significant role, various configurations would be important in realistic dissociative collisions. In this paper, we investigate the CID in He + H₂ with several different configurations. This is the simplest dissociative collision system in the sense that it has no rearrangement channel. The first study of CID in this system on a realistic potential energy surface (PES) has been made by Nobusada et al. using a standard close-coupling (CC) method [17,18]. They have considered a T-shape configuration, i.e., with the molecular orientation angle (represented by γ) relative to the intermolecular (He–H₂) axis being fixed to be π/2.
Unfortunately, they have found that the CC method requires a time-consuming calculation to obtain accurate dissociation probabilities especially at very high total energies \((E > 7.5 \text{ eV})\) or for very high vibrational states of \(\text{H}_2\) \((v > 9)\). Therefore, the CC method is not so useful to make an extensive study of the CID process. In this paper, instead of using the CC method, we employ a direct numerical method developed by Sakimoto and Onda \[19\]. In the latter method, the Schrödinger equation is directly solved on a grid of points in hyperspherical coordinates by means of the discrete variable representation \[21\]. As will be shown later, this method provides accurate results for all the vibrational states \((v = 0-14)\) in the energy range of \(E = 0-10 \text{ eV}\). In this study, we fix the orientation angle at \(\gamma = 0\) (collinear configuration), \(\pi/4\), and \(\pi/2\) (T-shape configuration), of which the last case is compared with the previous CC calculation \[18\].

2. Theory

2.1. Formulation

Let us introduce the Jacobi coordinates for the \(\text{He} + \text{H}_2\) system (Fig. 1). Here, \(r'\) and \(R'\) are the internuclear distance of \(\text{H}_2\) and the distance between \(\text{He}\) and the center-of-mass of \(\text{H}_2\), respectively. We assume that the orientation angle \(\gamma\) is constant during the collision. We define the mass-scaled coordinates as

\[
R = \left(\frac{4M}{M+2m}\right)^{1/4} R', \quad r = \left(\frac{4M}{M+2m}\right)^{-1/4} r',
\]

where \(M\) and \(m\) are the masses of \(\text{He}\) and \(\text{H}_2\), respectively. Then we have the Schrödinger equation for the \(\text{He} + \text{H}_2\) system in the form

\[
\left[-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial R^2} + \frac{\partial^2}{\partial r^2}\right) + V(R, r, \gamma)\right] \Psi(R, r) = E\Psi(R, r),
\]

where \(\mu = \sqrt{Mm^2/(M+2m)}\), and \(E\) is the total energy measured from the bottom of the \(\text{H}_2\) potential well. We employ the PES, \(V(R, r, \gamma)\), obtained by the \(\text{ab initio}\) calculation of Varandas and Brandão \[22\]. For \(\gamma = \pi/2\), it is the same one as is used in the CC study \[17,18\]. We show the contour maps of the PES for \(\gamma = 0, \pi/4,\) and \(\pi/2\) in Figs. 2a–2c.

Here, we introduce the hyperspherical coordinates \((\rho, \omega)\) defined by

\[
\rho = \sqrt{R^2 + r^2}, \quad \omega = \tan^{-1}\left(\frac{r}{R}\right).
\]

In the collinear collision \((\gamma = 0)\), the hyperangle \(\omega\) takes the value between 0 and \(\omega_{\text{max}} = \tan^{-1}\sqrt{(M+2m)/M}\). In the non-collinear collisions \((\gamma \neq 0)\), we assume that the helium atom does not go through the middle of the two hydrogen atoms (i.e., \(R\) is always non-negative), and hence the possible range of \(\omega\) becomes \((0, \omega_{\text{max}} = \pi/2)\). Since the motion along the \(\omega\) coordinate is always bounded, it is a great advantage to use the hyperspherical coordinates. Substituting Eq. (3) into Eq. (2) and representing the total wavefunction in the form \(\Psi = \rho^{-1/2}\eta(\rho, \omega)\), we have the partial differential equation

\[
\rho^2 \frac{\partial^2 \eta}{\partial \rho^2} + \frac{\partial^2 \eta}{\partial \omega^2} + W(\rho, \omega)\eta = 0,
\]

where

\[
W(\rho, \omega) = \frac{2\mu r^2}{\hbar^2} \left[E - V(\rho, \omega, \gamma)\right] + \frac{1}{4}.
\]

Eq. (4) can be solved using the direct numerical method of Sakimoto and Onda \[19\].

2.2. Scattering boundary condition

When the hyper-radius \(\rho\) is finite, the hyperspherical coordinates are not suitable for describing the asymptotic channels. This is because the hamiltonian for the asymptotic channels is not separable in hyperspherical coordinates as long as \(\rho < \infty\). For this reason, one encounters a difficulty in imposing a scattering boundary condition in hyperspherical coordinates. To avoid this problem, the wavefunction at sufficiently
large $\rho$ is often re-expanded in terms of the eigenfunctions in Jacobi coordinates [23]. However, this is not always possible when a dissociation channel becomes open [14,19,20]. Therefore, an approximation is usually needed to impose a scattering boundary condition for CID calculations [14,19,20]. In this work, we employ a scattering boundary analysis similar to the one developed by Sakimoto and Onda [19]. We separate the problem into two cases: the non-collinear ($\gamma \neq 0$) and the collinear ($\gamma = 0$) collisions.

### 2.3. Non-collinear ($\gamma \neq 0$) Collisions

We define the asymptotic region of $R > R_0$ in such a way that the $V(R, r, \gamma)$ becomes independent of $R$ and $\gamma$ there (Fig. 3). At $R > R_0$, we can write the wavefunction generally in the form

$$
\Psi_{\ell, e}(R, r, \gamma) = \Phi_{\ell, e}(r) \exp(-ik_{\ell, e}R)
+ \sum_{\ell', e'} \Phi_{\ell', e'}(r) \sqrt{\frac{k_{\ell'}}{k_{\ell'}}} \exp(ik_{\ell'}R) S_{\ell', e'}
+ \int d\epsilon \Phi_{\epsilon}(r) \sqrt{\frac{k_{\epsilon}}{k_{\epsilon}}} \exp(ik_{\epsilon}R) S_{\epsilon, e}.
\tag{6}
$$

Here, $\Phi_{\ell, e}(r)$ and $\Phi_{\epsilon}(r)$ are, respectively, the bound and continuum vibrational eigenfunctions of H$_2$. The suffix $\nu$ ($= 0$–14) is the vibrational quantum number, and $\epsilon$ is an eigenenergy of the dissociative continuum state. The wavenumbers $k_{\ell'}$ and $k_{\epsilon}$ are given in a usual way. The coefficients $S_{\ell', e'}$ and $S_{\epsilon, e}$ are the S-matrix elements.

![Schematic diagram for making the scattering boundary condition in non-collinear (\(\gamma \neq 0\)) configurations.](image-url)
To obtain the S-matrix elements, we should re-expand the numerical solution \( \rho^{-1/2} \psi(\rho, \omega) \) in the form of Eq. (6). However, this cannot be made for finite \( \rho \) because the numerical solution has a finite amplitude in the region of \( R < R_0 \) where the asymptotic form (6) is invalid. If \( \rho \to \infty \), the region of \( R < R_0 \) becomes negligible and hence we can determine the S-matrix elements uniquely. Unfortunately, the limit of \( \rho \to \infty \) is unreachable in numerical calculations. To make the calculation tractable, we impose a boundary condition in the following way. Let us denote the asymptotic region of \( r > r_0 \) in which no interaction works among the three atoms. First, as seen in Fig. 3, we make a numerical integration accurately in hyperspherical coordinates up to \( \rho = \rho_b \). Next, we choose some hyperangle \( \omega = \omega_b \) such that \( R_b = \rho_b \cos \omega_b > R_0 \) and \( r_b = \rho_b \sin \omega_b > r_0 \), and set an infinite wall along a line of \( r = r_b \) and \( R \geq R_0 \) and a line of \( R = R_b \) and \( r \geq r_b \). We assume that any atom cannot go into the domain of \( r \geq r_b \) and \( R \geq R_b \). This also means that the dissociative motion of \( \text{H}_2 \) is limited in the range of \( 0 \leq r \leq r_b \) at \( R \geq R_b \). In this way, instead of using Eq. (6), the numerical solution at \( \rho = \rho_b \) can be re-expanded in the form

\[
\Psi_v(R, r) = \varphi_v(r) \exp(-i\ell_v R) + \sum_{v'} \varphi_{v'}(r) \sqrt{\frac{k_{v'}}{k_v}} \exp(i\ell_{v'} R) A_{v'v},
\]

for \( R \geq R_b \),

\[
\Psi_v(R, r) = \sqrt{\frac{2}{R_b}} \sin \left( \frac{\nu \pi R}{R_b} \right) \sqrt{\frac{k_v}{k_{v'}}} \exp(i\ell_v R) b_{v'},
\]

for \( r \geq r_b \).

Here, \( \varphi_v \) for \( \nu = 0 - 14 \) is just equal to \( \phi_v \). The eigenfunctions \( \varphi_v \) of \( \nu \geq 15 \) describe the dissociative motion of \( \text{H}_2 \), and make a discrete set because the nuclear motion of \( \text{H}_2 \) is assumed to be bound in the way mentioned above. The eigenfunction of the motion along \( R \) at \( r \geq r_b \) is given by \( \sqrt{2/R_b} \sin(\nu \pi R/R_b) \), where \( \nu = 1, 2, \ldots \) indicates the discretized state in the region of \( r \geq r_b \). The coefficients \( A \) and \( B \) are just like the S-matrix elements. The dissociation probability for the initial vibrational state \( \nu \) can be given by

\[
\rho_{\text{diss}}^{\nu} = 1 - \sum_{\nu' = 0}^{14} |A_{\nu',\nu}|^2,
\]

where the sum in the right hand side is taken over all the bound states.

2.4. Collinear (\( \gamma = 0 \)) collision

In the collinear collision, it should be noted that Eq. (7) is no more valid as the asymptotic form because the interaction between \( \text{He} \) and \( \text{H} \) is not a separable form in the Jacobi coordinates \((r, R)\). However, it is evident that all the interactions at \( \omega \sim \omega_{\text{max}} \) and at large \( \rho \) are separable in an alternative set of Jacobi coordinates \((s, S)\) where \( s \) and \( S \) are the (mass scaled) distances of \( \text{He} + \text{H} \) and of \( \text{HeH} + \text{H} \), respectively. Since this situation is just the same as discussed by Sakimoto and Onda [19], we employ their boundary condition in the collinear case. Namely, we introduce a boundary parameter \( \omega = \omega_b \) and set an infinite wall along a line of \( r = r_b (= \rho_b \sin \omega_b) \) and \( R \geq R_b (= \rho_b \cos \omega_b) \) and of \( s = s_b (= \rho_b \sin(\omega_{\text{max}} - \omega_b)) \) and \( S \geq S_b (= \rho_b \cos(\omega_{\text{max}} - \omega_b)) \). Then, the asymptotic form for \( R \geq R_b \) \((0 \leq r \leq r_b)\) is just the same as Eq. (7a), and the one for \( S \geq S_b \) \((0 \leq s \leq s_b)\) is given in the Jacobi coordinates \((s, S)\). Since the details are shown in Refs. [19,20], we do not repeat them here.

3. Numerical accuracy

3.1. \( \omega_b \) dependence of the dissociation probabilities

In the present boundary analysis, we have introduced an artificial parameter \( \omega_b \). If the dissociation probability depends largely on \( \omega_b \), the present boundary condition is meaningless. We have examined the \( \omega_b \) dependence of the dissociation probabilities. Table 1 shows the dissociation probabilities for various values of \( \omega_b / \omega_{\text{max}} \) where \( \gamma = \pi/2 \), \( E = 8.0 \text{ eV} \), and \( \rho_b = 10 \text{ bohr} \). The table shows that the dissociation probabilities are almost independent of \( \omega_b \) (within about 1%) in a wide range of \( 0.4 \leq \omega_b / \omega_{\text{max}} \leq 0.7 \). If \( \omega_b \) is too close to zero or to \( \omega_{\text{max}} \), the condition of \( r_b > r_0 \) or \( R_b > R_0 \) cannot be satisfied. In the present case, we can obtain accurate dissociation probabilities when we take \( \omega_b \sim \omega_{\text{max}} / 2 \). In all the following calculations, we have set \( \omega_b = \omega_{\text{max}} / 2 \). For the integration
Table 1

<table>
<thead>
<tr>
<th>( \nu )</th>
<th>( \omega_0 / \omega_{\text{max}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>0.2931 0.4649 0.4640 0.4649 0.4657 0.4655 0.4654</td>
</tr>
<tr>
<td>0.35</td>
<td>0.2233 0.5583 0.5620 0.5616 0.5618 0.5608 0.5320</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5012 0.6693 0.6675 0.6676 0.6680 0.6640 0.6639</td>
</tr>
<tr>
<td>0.5</td>
<td>0.6594 0.7798 0.7917 0.7923 0.7924 0.7834 0.7576</td>
</tr>
<tr>
<td>0.6</td>
<td>0.7759 0.9368 0.9390 0.9409 0.9414 0.9407 0.9076</td>
</tr>
<tr>
<td>0.7</td>
<td>0.8</td>
</tr>
<tr>
<td>0.75</td>
<td>0.8</td>
</tr>
</tbody>
</table>

distance, we have taken \( \rho_b = 10 \) bohr for \( \gamma \neq 0 \) and \( \rho_b = 17 \) bohr for \( \gamma = 0 \). By these choices, the dissociation probabilities are always converged within \( 1\% \) with respect to \( \rho_b \).

3.2. Comparison with the CC method

To further check the numerical accuracy, Fig. 4 compares the present dissociation probabilities for \( \gamma = \pi/2 \) with those of the CC calculations [18]. We have obtained a satisfactory agreement with each other. This fact shows the reliability of the two calculations. In the CC method, the nuclear motion of \( \text{H}_2 \) is confined in a box with a size of \( r_{\text{max}} = 15.5 \) bohr, and the continuum channels are approximated by the discretized states in the box. Nobusada et al. have found that the box size of 15.5 bohr is not large enough to obtain accurate dissociation probabilities at higher energies \( (E > 7.5 \text{ eV}) \) or for higher vibrational states \( (\nu > 9) \) [18]. In Fig. 4, some of the probabilities converged with \( r_{\text{max}} = 15.5 \) bohr are shown for the CC calculation. On the other hand, the present study introduces the discretization approximation only in the boundary analysis, and the box size \( r_b \) is 9.03 bohr for \( \gamma \neq 0 \) and 9.31 bohr for \( \gamma = 0 \). It should be pointed out that the present calculation provides the converged results for all the vibrational states \( (\nu = 0–14) \) at the energies of \( E = 0–10 \) eV by these choices of \( r_b \), which are much smaller than the box size of 15.5 bohr in the CC calculation.

Fig. 4. Dissociation probabilities as a function of the total energy for \( \nu = 1, 3, 5, \) and 7 in the T-shape \((\gamma = \pi/2)\) configuration. The solid lines are the present results and the closed marks are the CC ones [18].

4. Results and discussion

Figs. 5a–5c show the dissociation probabilities in the energy range of \( E = 4.8–10 \) eV for the molecular orientations of \( \gamma = 0, \pi/4, \) and \( \pi/2, \) respectively. There are two significant differences among these three figures. (i) The onset of dissociation is strongly dependent on \( \gamma \): When \( \gamma = \pi/2 \), the dissociation is possible for all \( \nu \) at \( E > 7.5 \) eV. However, when \( \gamma = 0 \) and \( \pi/4 \), the dissociation probabilities have finite values only for very high vibrational states \( (\nu \geq 10) \). It seems that the dissociation occurs more easily for larger \( \gamma \). (ii) The dissociation probability curves have quite different features: The probabilities for \( \gamma = 0 \) are monotonically increasing with respect to \( E \) and indicate vibrational enhancement. When \( \gamma = \pi/4 \), the energy dependence becomes somewhat complicated since the probability curve has a local maximum at relatively low energies. When \( \gamma = \pi/2 \), the probability curves show undulation (except for \( \nu = 0 \)). The structure of undulation has been often found also
Fig. 5. Energy dependence of the dissociation probabilities for \( \gamma = 0, \frac{\pi}{4}, \) and \( \frac{\pi}{2} \).

Fig. 6. Adiabatic potential energy curves for \( \gamma = 0, \frac{\pi}{4}, \) and \( \frac{\pi}{2} \).

4.1. Adiabatic potential energy curves

In this study, we have used the hyperspherical coordinates in the numerical calculations. Although the present method does not need to calculate a set of adiabatic potential energy curves and non-adiabatic coupling matrix elements, an adiabatic picture is sometimes useful to understand the collision dynamics. Fig. 6 shows the adiabatic potential energies as a function of \( \rho \) for the present systems. The energy spacing among the adjacent potential curves becomes smaller with increasing \( \gamma \). This is because the possible range of \( \omega \) becomes wider for larger \( \gamma \) as shown in Fig. 2. Since smaller energy spacing makes non-adiabatic transition more significant, we can understand intuitively the tendency that the dissociation occurs more

in other studies [12,16,18,24]. Nobusada et al., using the classical S-matrix theory [25], have shown that the interference of two classical trajectories makes the undulation in the dissociation probability curves [18]. It should be pointed out that no clear undulation can be seen for \( \gamma = 0 \) and \( \frac{\pi}{4} \).

To obtain deeper insights of these CID dynamical features, we consider the problem first by seeing the hyperspherical adiabatic potential energies which are eigenvalues obtained by the diagonalization of the \( \omega \) motion for fixed \( \rho \), and next by examining the role of a kinematic factor due to mass combinations.
easily with increasing $\gamma$.

When $R'$ is varied but $r'$ is fixed, the He atom and one of the two H atoms have the closest distance at $R' = (r'/2) \cos \gamma$. Therefore, the He + $H_2$ PES has a barrier at this position and shows a double well structure along the $\omega$ coordinate as seen in Fig. 2b. Since we neglect the possibility of the He atom penetrating the $H_2$ molecule, no double well exists in the physically allowed region for $\gamma = 0$ or $\pi/2$. The barrier height of the double well decreases with increasing $\rho$. Owing to this double well structure, the adiabatic potential energy curves for $0 < \gamma < \pi/2$ have avoided crossing as shown in Fig. 6b. For $\gamma = \pi/4$, we can find the avoided crossing between the adiabatic curves of $v = 14$ and of the first continuum state at $E \sim 4.9$ eV, between $v = 13$ and 14 at $E \sim 5.5$ eV, between $v = 12$ and 13 at $E \sim 6.7$ eV, and so on. It should be noted that these energies almost correspond to the maximum peak positions of the dissociation probability curves each for $v = 14, 13, 12$, and so on. Therefore, the maximum peak of the dissociation probability at the low energies is evidently due to the avoided crossing. In the present case, the effect of the avoided crossing is drastic because the dissociation probabilities would be very small at the low energies if the avoided crossing is absent. It is interesting that the avoided crossing plays an important role even in the CID process.

4.2. Effects of mass combination on the dissociation

We have calculated the dissociation probabilities for $\gamma = 0$ and $\pi/2$ in the system of a $H-H-H$ mass combination ($M = m$) but on the PES of the He + $H_2$ system. In Fig. 7, the results for $v = 12$ are shown and compared with those for the original He–H–H case. There is a striking feature. When $\gamma = 0$, the probability becomes drastically large for changing the mass combination from He–H–H to H–H–H. However, when $\gamma = \pi/2$, the probabilities for the two mass combinations are not so different from each other. The mass kinematic factor plays a crucial role particularly in the collinear CID process. The effect of changing mass combinations was investigated in the collinear He+$H_2^+$ study by Dove and Mandy using the CT method [26]. Although He+$H_2^+$ system has a rearrangement channel, they obtained the same result that the dissociation probability increased in a large amount for the H–H–H mass combination. The present result further shows that in the H–H–H mass combination, the probabilities are not largely different for $\gamma = 0$ and $\pi/2$. This is in accord with the finding obtained by Rusinek and Robert in the semiclassical study of model $H + H_2$ collisions [24]. From these facts, we can expect that the collinear collision with the He–H–H mass combination has the dynamical feature distinct from the other cases.

There have been several CT studies that examine the kinematic role of mass combinations in atom–diatom collisions. Schinke and Toennies [27] have investigated the vibrational energy transfer in $H + H_2$ and He + $H_2$ collisions. In the collinear configuration, they found that the He impact was less effective for the vibrational excitation than the H impact. They further mentioned that for the He impact the incident atom had a chance of colliding with the recoiling $H_2$, i.e., a multiple collision, and for the H impact this phenomena rarely occurred. It had been well understood that the multiple collision made the vibrational excitation
inefficient by the deactivation of the target molecule [28]. In the T-shape configuration, Schinke and Toennies showed that there was no multiple collision leading to the deactivation for both the H and He impact [27]. In the CID process, Siré et al. [29], employing simplified collinear models, showed that the dissociation became inefficient in the presence of the multiple collision. Therefore, we can expect also in the present cases (shown in Fig. 5) that the multiple collision is important in the collinear He + H₂ configuration and hence the CID is relatively inefficient in this case.

As mentioned before, the undulation structure cannot be seen in the collinear He + H₂ collision (Fig. 5). However, in the model H + H₂ study, Rusinek and Roberts found the undulation both for the T-shape configuration and for the collinear one [24]. It seems that the multiple collision also affects the significance of the interference effect. When the multiple collision is less important such as in the H + H₂ or T-shape He + H₂ collisions, only two classical trajectories contribute to the classical S-matrix [18,24]. However, in the collinear He + H₂ configuration where the multiple collision occurs, probably more than two trajectories have the contribution. In this case, their interference effect is complicated, and hence the undulation structure is less conspicuous. When γ = π/4, since the PES has the barrier (Fig. 2b), the situation is somewhat similar to that in the collinear configuration. Therefore, for γ = π/4, the multiple collision would be important in the He + H₂ collision at least at low energies, and the undulation would not be seen well as in Fig. 5b.

5. Conclusion

We have studied the CID process in He + H₂ by using a direct numerical method of Sakimoto and Onda [19], which is much more efficient than a conventional CC method. We have introduced an approximation for the scattering boundary condition. Although this approximation is sufficient to obtain the total dissociation probabilities, it is highly desirable that a more accurate treatment will be developed.

As far as we know, the present work is the first quantum mechanical one that investigates the molecular-orientation dependence of CID. We have considered three orientations of γ = 0, π/4, and π/2. The CID occurs more easily for larger γ and shows strong γ dependence. In understanding the γ dependence, particularly important is the kinematic factor that the He mass is heavier than the H mass. Probably, the CID in H + H₂ does not have such strong γ dependence. The mass kinematic factor largely affects the visualization of the interference effect in CID as well. The adiabatic potential energy curve is also useful to understand the dynamics of CID. In particular, when 0 < γ < π/2, the adiabatic potential energy curves have avoided crossing, which plays a significant role in the low energy CID. The avoided crossing makes the γ dependence of the dissociation probability somewhat complicated.

Although it requires much more labour, the extension of the present calculation to 3D collisions by using an infinite-order-sudden approximation [30] is straightforward and very interesting.

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