CLASSICAL TRAJECTORY TREATMENT OF DIATOMIC MOLECULES
REACTING WITH SOLID SURFACES: A STUDY OF MASS EFFECTS

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The mechanism of the reaction between the diatomic molecule and a solid non-corrugated surface has been studied, employing the classical trajectory method. The study was performed in the energy range 1–6 eV, where all four types of collisions, inelastic, reaction (dissociative trapping), adsorption and dissociation, take place. To study mass effects three kinds of diatomic molecules were considered: the light-light (LL) mass combination represented by H₂, the light-heavy (LH) mass combination represented by HCl and HI and the heavy-heavy (HH) mass combination represented by Cl₂ and I₂. The main findings are: (a) The reactive process for the LL and HH systems is governed by one reaction mechanism, and those for the LH systems are governed by two different mechanisms. (b) Whereas the LL and HH systems tend to dissociate upon collision with the surface, once threshold for dissociation is reached no dissociation is encountered for the LH systems, even for energies of tens of electron volts. (c) The gas-solid-phase reactive process differs significantly from that encountered in the gas phase in that the important gas-phase quasicollinear arrangements play a negligible role in the gas-solid phase.

1. Introduction

Recently one of us (MB) presented a quantum-mechanical theory for treating an exchange (dissociative trapping) collision between a solid surface and a diatomic molecule [1]. This theory, based on the infinite order sudden approximation (IOSA), was transferred from the atom-diatom reactive case [2] and modified accordingly. Within this approach the following processes can be treated

\[ AB + S \rightarrow AB + S, \quad (Ia) \]
\[ \rightarrow AS + B, \quad (Ib) \]
\[ \rightarrow BS + A. \quad (Ic) \]

Here A and B are atoms and S stands for “surface”. Process (Ia) describes elastic or inelastic collisions, whereas the other two are exchange collisions. Two other processes which may occur are adsorption (which is the typical low-energy process):

\[ AB + S \rightarrow ABS \quad (Id) \]

and dissociation (which is the typical high-energy process):

\[ AB + S \rightarrow A + B + S. \quad (Ie) \]

An essential requirement of the relevance of reactive IOSA (RIOSA) [1] is the existence of a range of energies for which neither process (Id) nor process (Ie) occurs. Therefore, whether this rather strong requirement is met in realistic cases is an interesting question. To answer it we used the classical trajectory method [3–8]. In preliminary studies we found that one of the most important parameters relevant to this problem is the mass of the interacting particles. We treat three different mass combinations:

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(a) Two light atoms (the LL mass combination).
The typical diatomic for this case is $\text{H}_2$.
(b) One light atom and one heavy atom (the LH mass combination). $\text{HCl}$ and $\text{HI}$ were chosen to represent this case.
(c) Two heavy atoms (the HH mass combination). For this case $\text{Cl}_2$ and $\text{I}_2$ were selected.

We also study the extent to which the IOSA angle $\gamma$ (see fig. 1) is a “good” parameter to characterize final results. We present results as a function of the angle $\gamma$, to show the strong dependence of the various processes on this angle.

To make our results comprehensive and instructive, we chose to treat a surface which is rigid and non-corrugated. We are aware that this is a very unlikely situation, but we hope that at least some of our findings will apply to cases where the surface is quite rigid and the corrugation not too strong.

The reactions we treat [reactions (Ic)] are usually very endothermic and therefore the main emphasis will be on energies above 1–3 eV.

2. Description of the numerical treatment

The potential energy surface employed in this study is a modified LEPS surface as introduced by McCreery and Wolken [3]:

$$V = U_1 + U_2 + U_3$$

$$= \left[ Q_1^2 + (Q_2 + Q_3)^2 - Q_1(Q_2 + Q_3) \right]^{1/2},$$

where

$$U_i = \frac{D_i}{4(1 + \Delta_i)} \times \left\{ \begin{array}{l} \left[1 + (3 + \Delta_i^2) \exp\left[-2\alpha_i(r_i - r_{i0})\right] \right] \\ \left[-(2 + 6\Delta_i) \exp\left[-\alpha_i(r_i - r_{i0})\right] \right] \end{array} \right\},$$

and

$$Q_i = \frac{D_i}{4(1 + \Delta_i)} \times \left\{ \begin{array}{l} \left[1 + (1 + 3\Delta_i^2) \exp\left[-2\alpha_i(r_i - r_{i0})\right] \right] \\ \left[-(6 + 2\Delta_i) \exp\left[-\alpha_i(r_i - r_{i0})\right] \right] \end{array} \right\},$$

where $D_i$, $r_{i0}$ and $\alpha_i$ are the dissociation energy, the internuclear equilibrium distance and the characteristic Morse parameters, respectively. The coefficients $\Delta_i$ ($i = 1, 2, 3$) are the ordinary Sato parameters used to adjust the overall potential to have certain required features. Whereas the first three parameters are characteristic of each pair of particles, the Sato parameters have to be adjusted each time a different reaction is studied.

The various parameters employed in this study are summarized in tables 1 and 2. The parameters for the Morse potential of each diatomic were taken from ref. [9] and the parameters for the surface–H Morse potential were taken from ref. [10], assuming a metallic surface (nickel in this case). All other parameters were taken arbitrarily.

The results for several reactive systems presented were obtained from perpendicular trajectories started at a fixed initial distance with a given translational energy. In all cases the molecules are at $t = 0$, in their ground state, namely $v_i = j_i = 0$. 

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Table 1

Morse parameters for the various systems studied in this work

<table>
<thead>
<tr>
<th>Molecule</th>
<th>$D$ (eV)</th>
<th>$r_0$ (Å)</th>
<th>$D$ (Å$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$</td>
<td>4.746</td>
<td>0.7410</td>
<td>1.893</td>
</tr>
<tr>
<td>SH</td>
<td>2.74</td>
<td>1.65</td>
<td>1.025</td>
</tr>
<tr>
<td>HCl</td>
<td>4.613</td>
<td>1.277</td>
<td>1.865</td>
</tr>
<tr>
<td>SCl</td>
<td>1.5</td>
<td>2.014</td>
<td>1.887</td>
</tr>
<tr>
<td>Cl$_2$</td>
<td>2.517</td>
<td>2.00</td>
<td>2.01</td>
</tr>
<tr>
<td>HI</td>
<td>3.193</td>
<td>1.607</td>
<td>1.786</td>
</tr>
<tr>
<td>SI</td>
<td>1.00</td>
<td>2.20</td>
<td>1.887</td>
</tr>
<tr>
<td>I$_2$</td>
<td>1.550</td>
<td>2.666</td>
<td>1.866</td>
</tr>
</tbody>
</table>

$^a$ S indicates surface.
Table 2

<table>
<thead>
<tr>
<th>System[a)</th>
<th>Sato parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\Delta_1$ b)</td>
</tr>
<tr>
<td>H$_2$ + S → HS + H</td>
<td>0.03</td>
</tr>
<tr>
<td>HCl + S → HS + Cl</td>
<td>0.147</td>
</tr>
<tr>
<td>HI + S → HS + I</td>
<td>0.147</td>
</tr>
<tr>
<td>Cl$_2$ + S → ClS + Cl</td>
<td>0.0</td>
</tr>
<tr>
<td>I$_2$ + S → IS + I</td>
<td>0.03</td>
</tr>
</tbody>
</table>

a) S indicates surface.
b) Sato parameter for the diatomics.
c) Sato parameter for HS.
d) Sato parameter for halogen surface.

3. Results

3.1. Energy-dependent transition probabilities

In this study results are presented for five different systems classified in three categories:

5.1.1. The LL case

One system was studied, i.e.,

$\begin{align*}
H_2 + S & \rightarrow H_2 + S, \\
& \rightarrow HS + H, \\
& \rightarrow H_2S, \\
& \rightarrow 2H + S.
\end{align*}$

The transition probabilities as a function of total energy are presented in fig. 2a. Since our main interest is in the reaction (exchange) process which starts (due to the endothermicity) at high energies, we usually concentrate on the relevant energy range. In this particular case, the threshold is around 4 eV. In order to see how the various thresholds, obtained from the classical trajectory study, are related to the theoretical (lowest) thresholds, the latter are summarized in table 3. (The values in table 3 are differences in the corresponding $D$ values.) The theoretical thresholds are seen to be usually much lower than the calculated ones; the calculated threshold for reaction (IIb) is $\approx 2.0$ eV higher (see table 4) and the threshold for dissociation is 0.7 eV higher (5.50 versus 4.77 eV).

From fig. 2a it can be seen that along the whole energy range not one single energy value exists for which the reaction (exchange collision) is the only chemical process. In the lower-energy range (from threshold up to 6.5 eV) the reactive process mainly

Table 3

| Threshold (total) energies for the various processes (eV). (S indicates surface) |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|
|                                  | $A + SB$        | $B + SA$        | $ABS$           | $A + B + S$     |
| H$_2$ + S                        | 2.034           | 2.034           | -0.706          | 4.774           |
| HCl + S                          | 1.875          a) | 3.115           | +0.375          | 4.615           |
| HI + S                           | 0.453          a) | 2.499           | -0.241          | 3.193           |
| Cl$_2$ + S                       | 1.017           | 1.017           | -0.483          | 2.517           |
| I$_2$ + S                        | 0.550           | 0.550           | -0.450          | 1.550           |

a) B is the hydrogen atom.
Fig. 2. Transition probabilities as a function of total energy for the systems (a) H₂ + S; (b) Cl₂ + S; (c) I₂ + S; (d) HCl + S; (e) HI + S, and (f) H₂S + S, for (---) $D_{st1} = 1.0$ eV and (- - -) $D_{st1} = 0.7$ eV. (○) Adsorption probability; (□) reaction probability; (×) dissociation probability; (+) inelastic transition probability.

Table 4
Comparison between theoretical and calculated (see fig. 2) thresholds (eV) for the reaction $AB + S \rightarrow BS + A$

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Theoretical</th>
<th>Calculated</th>
<th>Difference absolute</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂ + S</td>
<td>2.034</td>
<td>≈ 4.0</td>
<td>≈ 2.0</td>
<td>100</td>
</tr>
<tr>
<td>HCl + S</td>
<td>1.875</td>
<td>≈ 2.0</td>
<td>≈ 0.125</td>
<td>7</td>
</tr>
<tr>
<td>HI + S</td>
<td>0.453</td>
<td>≈ 0.6</td>
<td>≈ 0.147</td>
<td>32</td>
</tr>
<tr>
<td>Cl₂ + S</td>
<td>1.017</td>
<td>≈ 2.0</td>
<td>≈ 1.0</td>
<td>100</td>
</tr>
<tr>
<td>I₂ + S</td>
<td>0.550</td>
<td>≈ 1.0</td>
<td>≈ 0.45</td>
<td>82</td>
</tr>
</tbody>
</table>

interferes with adsorption [reaction (IIc)] and in the higher-energy range (starting at 5.5 eV) it interferes with dissociation. Another notable feature is the absence of inelastic or elastic collisions.

3.1.2. The HH case

Two systems were studied:

$$X_2 + S \rightarrow X_2 + S,$$  (IIIa)
$$\rightarrow XS + X,$$           (IIIb)
$$\rightarrow X_2S,$$              (IIIc)
$$\rightarrow 2X + S,$$            (IIIId)
where X = Cl, I. The transition probabilities for all four processes are shown in figs. 2b and 2c and the corresponding theoretical thresholds are given in tables 3 and 4. For Cl₂ the theoretical thresholds are seen to be \( \approx 1 \text{ eV} \) lower than the actual thresholds (1.0 versus 2.0 eV for reaction and 2.5 versus 3.5 eV for dissociation).

Also here, like in the previous LL case, the reaction process overlaps, over the entire energy range, either with adsorption (in the lower-energy interval) or with dissociation (in the higher-energy interval). However, the situation here is somewhat more relaxed; the adsorption and dissociation seem to interfere over a much smaller energy range than in the LL case. In fact, in the I₂ case there may even exist a short energy range (around 1.7 eV) where the two processes do not overlap at all, and consequently the only chemical process occurring in that range is the reaction.

### 3.1.3. The LH case

Two systems were studied:

\[
\begin{align*}
\text{HX} + \text{S} & \rightarrow \text{HX} + \text{S}, \\
& \rightarrow \text{HS} + \text{X}, \\
& \rightarrow \text{XS} + \text{H}, \\
& \rightarrow \text{HXS}, \\
& \rightarrow \text{H} + \text{X} + \text{S},
\end{align*}
\]

where X = Cl, I. The transition probabilities for HCl and HI are given in figs. 2d, 2e and 2f, respectively. The calculations for HI were made for two different \( D \) values. The results for \( D = 1 \text{ eV} \) (the tabular value) are presented in fig. 2e, and in fig. 2f the adsorption and the reaction transition probabilities are compared with those obtained with a lower \( D \) value, i.e., \( D = 0.7 \text{ eV} \).

The two HX systems differ from the previous systems because here two reaction products, i.e., HS and XS (X = Cl, I) are expected. However, as can be seen from table 3, the threshold for XS production are much higher, and in the actual calculation these products are not encountered, even for energies as high as 6 eV. Consequently, no reference is made to this possibility.

The two LH systems differ significantly from each other. In the HCl case, large inelastic (or elastic) transition probabilities are encountered in the low-energy region, causing the adsorption to be less pronounced. In the HI case the inelastic process is rarely encountered, enhancing the probability of adsorption in the low-energy range (and of reaction in the higher-energy range). The reason is that in the HCl case the adsorption is an endothermic process (see table 3) and in the HI case it is an exothermic process. The difference in bonding energies between the two halogens and the surface also explains why the adsorption probability decreases faster for HI; the difference is 0.5 eV in favor of SCl (see table 1).

The adsorption and reaction transition probabilities for HI as calculated with two different \( D_\text{st} \) values, i.e., \( D_\text{st} = 1.0 \) and 0.7 eV (all other parameters are unchanged) are compared in fig. 2f. Reducing \( D_\text{st} \) from 1.0 to 0.7 eV causes the adsorption probability to decrease faster and the reaction probability function to increase at the same rate, as a function of energy. The explanation is as follows. The adsorption becomes less probable because the binding energy between the iodine and the surface is decreased. The adsorption and the reaction processes are closely related because in both cases the molecule dissociates; however, in the former process, the iodine is captured on the surface and in the latter it is not. Thus, due to weakening of the adsorption, the reaction is enhanced.

The LH systems differ significantly from the LL and HH systems, in two major features:

(a) The differences between the theoretical and calculated threshold energies for the exchange reactions (I). From the comparison in table 4 it is seen that these differences are much smaller for the reaction \( \text{HX} + \text{S} \rightarrow \text{HS} + \text{X} \). The explanation for this phenomenon is as follows: for a reaction to take place, the two atoms, while approaching the surface, must move away from each other fast enough to prevent their recombining when subsequently retreating from the surface. This requirement is best fulfilled for the LH case, where the light hydrogen manages to be far from the heavy iodine (or chlorine) as it starts to leave the surface. In the other cases, either two light atoms or two heavy atoms are encountered and therefore the adsorbed atom does not always manage to be
beyond the scope of attraction of the other atom before the latter leaves the surface.

(b) In contrast to the LL and HH systems, for the LH system dissociation is not encountered, even for energies as high as tens of electron volts. (The theoretical values for the LH systems are relatively low, around 3–5 eV.) In order to explain this finding we suggest using a “free spectator” model within which a two-step dissociation is assumed to take place:

(i) The approaching molecule dissociates on the surface and the two free atoms move on the surface with the following components of energy: a horizontal energy which is mainly due to the original vibrational motion and a perpendicular energy which is mainly due to the original translational motion and remains almost unchanged. If \( E_i \) is the initial (perpendicular) translational energy and \( \Delta H \) is the endothermicity for adsorption of the two atoms, then the partitioning of the perpendicular energy between the two atoms is according to:

\[
E_x = \left[ m_x / (m_x + m_y) \right] (E_i - \Delta H),
\]

where \( m_x \) and \( m_y \) are the masses.

(ii) The two atoms leave the surface. The conditions for that are:

\[
E_x > D_x, \quad E_y > D_y,
\]

or

\[
E_x > \Delta H + (m_x + m_y) \max\left( D_x/m_x, D_y/m_y \right),
\]

where \( D_x \) and \( D_y \) are the respective binding energies.

Eq. (6) yields the theoretical values for the case where the two masses are equal. Thus, within the model dissociation threshold energy values are equal to the theoretical values shown in the fifth column of table 3. However, different values are obtained when \( m_x \neq m_y \). For HCl and HI, eq. (6) yields values of 98 and 350 eV, respectively. This explains why dissociation is absent from our calculations.

3.2. Transition probabilities as a function of the angle \( \gamma_0 \)

The angle \( \gamma_0 \) (see fig. 1) is one of the initial values (usually randomly selected) for which approximations can be made. Consequently it could be of importance to study the dependence of certain probabilities on this parameter.

Various transition probabilities for HCl as a function of \( \gamma_0 \), and for different energies are shown in fig. 3. (It should be noted that when \( 0 < \gamma_0 < \pi/2 \), the H atom is closer to the surface.) Although \( \gamma \) is a variable that changes with time, meaningful conclusions can be drawn from the \( \gamma_0 \)-dependent histograms. It is seen that the main contributions to the reaction probabilities are from \( \gamma_0 \) larger than \( \pi/2 \) (in the lower-energy region all contributions are from this region). However, it is noted that as \( E_{\text{tot}} \) increases, more and more contributions come from the \( \gamma_0 < \pi/2 \) region. In fact, for \( E_{\text{tot}} = 4.5 \) eV (not shown in the figure), the reaction probability is 0.95, which means that almost every value of \( \gamma_0 \) (except \( \gamma_0 \approx \pi \)) leads to reaction. Sometimes, as the energy is increased, a peculiarly discontinuous behavior is encountered. Such is the case for \( E_{\text{tot}} = 2.75 \) eV, where neither reaction nor adsorption takes place when \( 60^\circ < \gamma < 90^\circ \), or the case of \( E_{\text{tot}} = 3.0 \) eV, where unexpectedly large reaction probabilities are obtained for small \( \gamma_0 \) values (\( 0^\circ \leq \gamma_0 \leq 30^\circ \)).

To get some more insight into the reaction mechanism, we decided to study a reactive trajectory in more detail. The interatomic distances, i.e., \( r_{\text{HCl}}(t) \), \( r_{\text{H}}(t) \) and \( r_{\text{C}}(t) \) as well as \( \gamma(t) \) are presented for \( E_{\text{tot}} = 2.75 \) eV and \( \gamma_0 = 40^\circ \) in fig. 4, and for \( E_{\text{tot}} = 3.5 \) eV and \( \gamma_0 = 85^\circ \) in fig. 5. Whereas the curves for the interatomic distances in figs. 4a and 5a seem rather similar, significant differences are noticed with regard to \( \gamma(t) \). In fig. 4b, \( \gamma(t) \) increased from \( \gamma = 40^\circ \) to \( \approx 270^\circ \), whereas in fig. 5b, \( \gamma(t) \) increases from \( 85^\circ \) to \( 145^\circ \), then decreases back to \( \approx 90^\circ \). Thus, although the final products are the same in the two cases, namely, a free chlorine and an adsorbed hydrogen, the reaction coordinates are different. More details on the two types of reaction coordinates can be found in ref. [11].

From tracing a large number of trajectories, the following conclusions can be drawn:

(a) The type of trajectories shown in fig. 4 are typical only for low \( \gamma_0 \) (\( \leq 60^\circ \)) and for low energies (\( E_{\text{tot}} \leq 3.0 \) eV).

(b) The type of trajectories shown in fig. 5 are
Fig. 3. Transition probabilities as a function of the initial value of $\gamma$ as calculated for the HCl+S system for different energies. Inelastic, reaction and adsorption transition probabilities are shown.

Fig. 4. Reactive trajectory for the HCl+S system as calculated for $E_{\text{tot}} = 2.75$ eV and (initial) $\gamma_0 = 40^\circ$. (a) Interatomic distances as a function of time: (-----) $r$(HCl); (-----) $r$(HS); (----) $r$(CIS). (b) The angle $\gamma$ as a function of time.
much more common and are encountered in all other cases.

These facts being known, we are able to explain part of the findings regarding the discontinuity encountered in the \( \gamma_0 \)-dependent histograms for \( E_{\text{tot}} = 2.75 \) and \( 3.0 \) eV. Thus, the low \( \gamma_0 \) reaction probabilities for these energy values are due to the former mechanism [mechanism (a)], whereas those for the high \( \gamma_0 \) are due to the latter mechanism. The fact that, for instance, at \( E_{\text{tot}} = 2.75 \) and \( 60^\circ \leq \gamma_0 \leq 90^\circ \) no reaction takes place just means that the two kinds of mechanisms do not overlap.

\( \gamma_0 \)-dependent histograms for \( \text{H}_2 \) and \( \text{Cl}_2 \) are shown in figs. 6a and 6b, respectively. For each case we chose two energies, the first in the vicinity of the reaction threshold and the other in the vicinity of the dissociation threshold (which is also close to the energy region where the adsorption decays to zero). Histograms for adsorption, reaction and dissociation are shown. (Inelastic transition probabilities are not presented because they are either zero, like in the \( \text{H}_2 \) case, or relatively small, as in the \( \text{Cl}_2 \) case.) From fig. 6a it is seen that for \( \text{H}_2 \) in the reaction threshold region, a
strong $\gamma_0$-dependence is encountered; the reaction is quite probable for $\gamma_0 < 60^\circ$ (or $\gamma_0 > 120^\circ$) but not possible at all for $60^\circ < \gamma_0 < 120^\circ$. This selectivity is diminished when the energy is raised to 6 eV, although the $60^\circ < \gamma_0 < 120^\circ$ region is still less probable. It can also be seen that dissociation starts when the molecule approaches the surface while remaining parallel to it ($60^\circ < \gamma_0 < 120^\circ$).

Another point about H$_2$ is that the reacting H (namely the H that stays on the surface following the collision) is always the one that was originally farther from the surface.

Fig. 6b shows that the reaction probabilities are only weakly dependent on $\gamma_0$. A stronger dependence (at least around threshold) is obtained for dissociation, where the $60^\circ < \gamma_0 < 120^\circ$ region is favored. Fig. 7 shows the probability distribution for a certain Cl atom to react. Thus, unlike in the H$_2$ case, the closer Cl is more likely to react than the further one.

We also considered trajectories as a function of time for both the H$_2$ molecule and the Cl$_2$ molecule, but none of the interesting features encountered with the HCl were seen here. In other words, the more common mechanism for reaction for HCl (that where $\gamma$ never becomes larger than $180^\circ$) is the only mechanism governing the reaction of H$_2$ and Cl$_2$ with the surface.

### 4. Conclusions

In this work we studied mass effects which result from the interaction of diatomic molecules with solid, non-corrugated surfaces in the energy range of 1–6 eV. Three types of cases were considered: the LL case, represented by H$_2$, the HH case, represented by Cl$_2$, and the LH case, represented by HCl and HI. The four types of possible processes, i.e., inelastic, adsorption, reaction and dissociation, were analyzed, but particular emphasis was put on the reaction process. It was found that the LH interaction differs significantly from the HH and the LL interactions, in two ways:

(a) Whereas the reaction process for LL and HH is governed by one mechanism which follows one typical reaction coordinate, the reaction process for the LH systems is governed by two types of mechanisms, which follows two different reaction coordinates.

(b) Whereas the LL and HH systems tended to dissociate once the energy was in the vicinity of the dissociation threshold, no dissociation was encountered for the LH systems, even for energies as high as tens of electron volts.

It is important to compare the reaction mechanism in the gas–solid phase with that in the gas phase. It is known from many studies on the gas phase that arrangements in the vicinity of the collinear arrangement, where the reacting atom faces the reagent atom, have a much higher probability of leading to reactions than other arrangements. This is altogether different in the gas–solid phase. Here in most cases the farther atom is more likely to be adsorbed on the surface.

The research described in this work was carried out on a fast and non-dissipative surface and the realism of the findings is therefore open to question. There is no doubt that adding corrugation will affect the results of the LL systems, that it will have no effect on the HH results and that it might affect the LH results to a certain extent. Making the surface dissipative will not affect the LL systems, but might affect the HH and the LH systems.

In general we expect that introducing dissipation and corrugation into our calculations might shift the thresholds for some of the processes and
might enhance or diminish some of the probabilities, but no essential changes are expected to appear. The main findings of this study, those related to the LH systems in particular, will definitely not be severely affected by these modifications. We are now in the process of introducing these features into our classical trajectory programs and we hope to be able to study this problem in the near future.

References