Collinear study of protonium formation in collisions of antiprotons with hydrogen molecular ions

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Abstract

Applicability of the Born–Oppenheimer adiabatic approximation is examined for the protonium formation process \( \bar{p} + H_2^+ \rightarrow \bar{p}p + H \). For this purpose, a collinear configuration is assumed for the three nuclei, and a calculation using a quantum–classical hybrid (semiclassical) method is carried out. The collinear study suggests that the molecular target is much more efficient for the production of the protonium atom than the target of atomic hydrogen.

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1. Introduction

In collisions between antiprotons (\( \bar{p} \)) and H atoms, the protonium formation (\( \rightarrow \bar{p}p + e \)) is significant only at energies less than the ionization limit (13.6 eV) [1, 2]. Above the ionization limit, the protonium formation hardly occurs, and the breakup ionization (\( \rightarrow \bar{p} + p + e \)) becomes the dominant reaction channel. This is because the antiproton and the electron have large mass difference, and the momentum transfer between the two particles is inefficient. Recently, Cohen [3] studied the protonium formation in \( \bar{p} + H_2 \) by using a fermion molecular dynamics (FMD) method. He found that the protonium formation had the cross section larger than that for the H atom target, and was induced at energies much higher than 13.6 eV. The molecular target seems to make the protonium formation more efficient.

In this study, we consider the protonium formation in collisions between antiprotons and \( H_2^+ \) molecular ions

\[
\bar{p} + H_2^+ \rightarrow \bar{p}p + H. \tag{1}
\]

When the system is composed of an antiproton and a positive ion, previous studies [4, 5] suggested that the Born–Oppenheimer (BO) approximation worked nicely to describe the electronic state. The BO approximation is very familiar in the chemical reaction studies. In this paper, we examine the applicability of the BO approximation for the process (1). For this purpose, we solve the quantum equation of the electronic motion in a numerically accurate manner. Unfortunately, a complete quantum mechanical description is not so easy for the four-body system. Hence, we employ a quantum–classical hybrid (QC) method, in which the electron is treated in quantum mechanics and the
heavy nuclei (the antiproton and two protons) are in classical mechanics. The QC method has been used to study $\mu^- + H \rightarrow \mu^- p + e$ [6] and $p + H \rightarrow pp + e$ [7]. Its applicability has been discussed elsewhere [8–10].

We further assume a collinear configuration for the three nuclei. Collinear studies have been frequently performed to understand the chemical reaction dynamics. Here, the collinear assumption is expected to be very useful for testing the BO approximation. This work is also preliminary to the three-dimensional (3D) treatment.

2. Theory

We consider the collinear configuration arranged in order of $p$–$p$–$p$. We describe the positions of the three nuclei in Jacobi coordinates $(R, r)$, where $r$ is the distance between the two protons and $R$ is the distance between the antiproton and the midpoint of $r$. The position vector of the electron is represented by $s$, and the distances to the electron from the outer and inner protons and the antiproton are represented by $s_1$, $s_2$ and $s_3$, respectively. Atomic units are used unless otherwise stated.

2.1. BO approximation

First, we consider the BO approximation. The BO state is obtained by

$$H_0 \Theta(s) = \epsilon_{BO}(R, r) \Theta(s),$$

where $H_0$ is the electronic Hamiltonian

$$H_0 = -\frac{1}{2} \nabla_s^2 - \frac{1}{s_1} - \frac{1}{s_2} + \frac{1}{s_3}$$

and $\epsilon_{BO}$ is the adiabatic energy of the electron. Then, as usually done in the chemical reaction studies, we may introduce the potential energy surface (PES) for the three-body system $H$–$p$–$p$ as

$$V_{PES}(R, r) = \epsilon_{BO}(R, r) + V_{\text{nuclei}}(R, r),$$

where

$$V_{\text{nuclei}}(R, r) = \frac{1}{r} - \frac{1}{R + r/2} - \frac{1}{R - r/2}$$

$$+ \frac{L(L + 1)}{2m(R - r/2)^2},$$

is the interaction among the three nuclei. In the collinear configuration, because the direct encounter always occurs between the antiproton and the inner proton, the singularity of the attractive Coulomb interaction causes some instability in the numerical calculation. To avoid this, we have added the centrifugal potential in the nuclear interaction. In the centrifugal term, $m$ is the reduced mass of $p + p$ and $L$ can be regarded as the angular momentum quantum number of the $pp$ atom.

In the BO approximation, the Hamiltonian for the the nuclear motions is given by

$$H_{BO} = \frac{1}{2\mu} p_r^2 + \frac{1}{m} p_r^2 + V_{\text{PES}}(R, r),$$

where $\mu$ is the reduced mass of $p + H^+_2$. To describe the heavy nuclear motions, we employ classical mechanics.

2.2. QC method

In the QC method, we introduce the following classical quantity at each time $t$:

$$H_{QC} = \frac{1}{2\mu} p_r^2 + \frac{1}{m} p_r^2 + |\Psi[H_0]|\Psi\langle\Psi|\Psi\rangle^{-1}$$

$$+ V_{\text{nuclei}}(R, r),$$

where $\Psi(s, t)$ is the time dependent wavefunction of the electronic state, and is given by solving the time-dependent Schrödinger equation,

$$i \frac{\partial}{\partial t} \Psi(s, t) = H_0 \Psi(s, t).$$

We regard the quantity (7) as a classical Hamiltonian, and use it to provide the nuclear trajectories $R(t)$ and $r(t)$. It should be noted that Eq. (7) becomes just identical to (6) if the BO approximation is very good.

In the calculation of the electronic state (8), we use the discrete-variable-representation (DVR) method [11,12]. To take account of the two-center Coulomb nature of the $H^+_2$ molecule, we need to introduce spheroidal coordinates [13]. For the details of the numerical calculation, see [14]. The solution in this way can cover an accurate description of the electronic excitation and also the ionization.
3. Results

Fig. 1 shows a contour plot of the PES for \( L = 60 \) obtained in the BO approximation. The valleys at \( r \approx 2 \) a.u. and along \( R \approx r/2 \) correspond, respectively, to the reagent channel \((\text{p} + \text{H}_2)\) and to the product channel \((\text{pp} + \text{H})\). The plateau with energies of \( \approx -0.5 \) eV is located where both the distances \( r \) and \( |R - r/2| \) are large. The scattering to this area corresponds to the dissociation \((\text{p} + \text{p} + \text{H})\).

To see to what extent the electronic excitation is important, we calculate the occupation probability of the electronically ground state after the collision:

\[
P_{\text{gs}} = \left| \langle \Theta | \Psi(t = \infty) \rangle \right|^2 \langle \Psi(t = \infty) | \Psi(t = \infty) \rangle^{-1},
\]

where the BO wavefunction \( \Theta \) is given by setting \( R = R(t = \infty) \) and \( r = r(t = \infty) \). Fig. 2 shows the occupation probabilities at collision energies up to 300 eV. We can see that the probability deviates from unity with increasing energies, but is still very close to unity. Therefore, the electronic excitation is certainly negligible at energies below a few hundreds eV.

Finally, in Fig. 3, the final energies \( E_{\text{pp}} \) of the \text{pp} atom for \( L = 60 \) are plotted against the initial angle variable of the molecular vibration. The results are obtained by the BO approximation and the QC method for the collision energy of 200 eV. The negative value of \( E_{\text{pp}} \) means that the \text{pp} atom is produced by the collision. We can obtain a good agreement between the two calculations. Therefore, the BO approximation is very nice for the calculation at least for energies below a few hundreds eV. This is highly encouraging for performing the 3D calculation because the four-body problem can be reduced to the three-body collision on the BO surface.
When the energy is very high ($\gtrsim 1$ keV), the electronic excitation or ionization becomes important [14]. The QC method will be still useful for studying the reactions including such electronic processes. We are very interested in $p + H_2$. The FMD study [3] showed that the dominant channel for protonium formation was $p + H_2 \rightarrow pp + H + e$. For the $H_2$ molecule target, hence we will have to consider the ionization accurately. This case is just suitable for the application of the QC method.

References


