Ionization of atomic hydrogen and He$^+$ by slow antiprotons

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Abstract. We study the ionization process involving antiproton ($\bar{p}$) and hydrogen in the energy range between 0.1 keV to 500 keV, using single center close coupling approximation. We construct the scattering wave function using B-spline bases. The results obtained for ionization of atomic hydrogen are compared with other existing theoretical calculations as well as with the available experimental data. The present results are found to be encouraging. We also employed this method to study the ionization of He$^+$ in the energy range between 1 and 500 keV. On comparison, the present results are found to interpret well the cross section values calculated using other theories.

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1. Introduction

The recent experimental research using slow antiprotons ($\bar{p}$) has been in progress. In near future it will measure the cross sections in the low energy region and will provide a strong challenge to theory in order to predict accurate cross sections in the energy range the experiment is concerned. The collisions of $\bar{p}$ with atomic hydrogen can be considered as a fundamental process and is relevant in many applied areas of physics. For proton impact, the final state can be a superposition of elastic scattering, excitation, ionization and charge exchange. However, for antiproton impact the charge transfer channel is absent. Despite this simplicity, this process needs a careful treatment especially in the case of slow $\bar{p}$ projectile. In low energy heavy particle collision it is not easy to single out the dominant channel, because many inelastic channels strongly couple with one another open up, exchanging flux and phase in complicated manner. Thus without inclusion of important channels, an accurate determination of cross sections is not possible. In case of ionization it is particularly important to describe the continuum part of the wave function with utmost care in order to achieve accurate results.

Recently, there have been a large number of studies for $\bar{p}$-H system using various theoretical approaches. However, most of the close coupling calculations are concentrated on single center expansion method. It has been realized that accurate cross sections can be calculated if a single-centred basis includes states with high angular momenta. Because states associated with high angular momenta are capable of describing the two center nature of the collision processes and is particularly suitable for $\bar{p}$ scattering (Hall et al 1994, 1996, Wherman et al 1996). However, it has been reported by Toshima (2001) that below 1 keV the one center pseudostate expansion method underestimates the cross sections due to inability to represent the expanding distribution of ionized electrons. For $\bar{p}$ projectile, most of the calculations performed are single center close coupling methods, based on semiclassical impact parameter treatment where the scattering wavefunctions are expanded around the target nucleus using suitable bases (Schwietz 1990, Hall et al 1996, Igarashi et al 2000, Azuma et al 2002). Pons (1996) proposed a new monomeric close coupling expansion in terms of spherical Bessel functions confined in a finite box in the study of $\bar{p}$ - H ionization. Other methods include direct solution of Schrödinger equation: Wells et al (1996) solved the Schrödinger equation directly on three dimensional lattice without using expansion of basis set. Similarly Tong et al (2001) solved the Schrödinger equation taking a semiclassical approximation for nuclear motion and the time evolution of electron wave function is propagated by split-operator method with generalized pseudospectral method in the energy representation. Sakimoto (2000) solved the time dependent Schrödinger equation directly using a discrete variable representation technique. For radial coordinates, he constructed the numerical mesh from generalized laguerre quadrature points.

In this article we make use of B-spline bases for the construction of scattering wave function. B-spline has been widely used in atomic physics (Martrin 1999) particularly due to its ability to describe the continuum channels more accurately in comparison to
other conventional methods (Azuma et al 2002). We give particular interest to study the ionization of He$^+$ under $\bar{p}$ impact. For the collision of $\bar{p}$ with hydrogenic ions such as He$^+$, a number of calculations have been performed. Schultz et al (1996a) used four different methods to calculate the cross sections: very large scale numerical solution of time-dependent Schrödinger equation (TDSE), hidden crossing theory (HC), classical trajectory Monte Carlo (CTMC), and continuum distorted eikonal initial state (CDE-EIS). TDSE calculations which are assumed to be the most accurate in the low energy region are found closer to HC results at low energies. This calculation also follows CTMC results at intermediate energies and CDW-EIS results at high energies. However, the TDSE cross sections are found to be about four times larger than those calculated by Janev et al (1995). A discussion about this disagreements can be seen in the article by Krstic et al (1996). Wherman et al (1996) used a large single centred Hibert basis sets to study the ionization of He$^+$ by antiproton impact. They found that their results are in good agreement with TDSE results, differing by 6-13% and the results obtained by Janev et al (1995) were smaller by a factor of four. Kirchner et al (1999) used basis generator method (BGM) for $\bar{p}$ - He$^+$ ionization. In case of $\bar{p}$ - H system, there is good convergency of results among various theoretical approaches. However, the experimental data in the low energy range is awaited. For the case of $\bar{p}$ - He$^+$ ionization there is no experimental data available and it is necessary to investigate this system in detail using different approaches and compare the results with other theories. We study the ionization process of hydrogenic ions under slow $\bar{p}$ projectile impact using single center expansion of scattering wave function in terms of B-spline basis sets. The detailed description of present theory is presented in section II. Atomic units (a.u.) are are used throughout unless otherwise stated.

2. Theory

We use impact parameter approximation where the internuclear motion is treated classically as $\mathbf{R} = \mathbf{b} + \mathbf{v}t$, with $\mathbf{b}$ the impact parameter, $\mathbf{v}$ the impact velocity and $t$ the time and the electronic motion is subjected to quantum mechanical laws. The electronic motion can be described by the solution of time dependent Schrödinger equation

$$\left( H_0 + V_{int} - i \frac{\partial}{\partial t} \right) \Psi(\mathbf{r}, \mathbf{R}) = 0$$

(1)

where $\mathbf{r}$ is the position vector of the electron with respect to proton. The atomic Hamiltonian is defined as

$$H_0 = -\frac{1}{2} \nabla^2 - \frac{Z_T}{r_T}$$

(2)

where $Z_T$ is the nuclear charge of the target and $V_{int}$ is the time dependent interaction between the projectile and target electron. The interaction between $\bar{p}$ - hydrogenic ions is given by

$$V_{int} = \frac{1}{|\mathbf{r} - \mathbf{R}|}$$

(3)
The total wave function is expanded as
\[ \Psi_{n\ell m}(r) = \sum_{n\ell m} a_{n\ell m}(t) \phi_{n\ell m}(r)e^{i\varepsilon_{n\ell m}t}, \]  (4)
where \( B^k_i(r) \) is the k-th order B-spline functions. The entire space of the electron sphere is confined with radius \( r = r_{\text{max}} \). The interval \([0, r_{\text{max}}]\) is then divided into segments. The end points of these segments are given by the knot sequence \( t_i, i=1,2,\ldots,n+k \). B-splines are piecewise polynomials of order k defined recursively on this knot sequence via the formula:
\[ B^1_i(r) = \begin{cases} 1 & t_i \leq r < t_{i+1} \\ 0 & \text{otherwise} \end{cases}, \]  (7)
and
\[ B^k_i(r) = \frac{r-t_i}{t_{i+k-1}-t_i} B^{k-1}_i(r) + \frac{t_{i+k}-r}{t_{i+k}-t_{i+k}} B^{k-1}_{i+1}(r). \]  (8)

Each B-spline is a piecewise polynomial of degree \( k-1 \) inside the interval \( t_i \leq r < t_{i+1} \) and zero outside the interval. The piecewise nature of B-splines are ideally suited to represent atomic wave functions. We chose an exponential knot sequence so as to model the exponential behaviour of the wavefunctions. For the radial function to satisfies the boundary condition that \( F_{n\ell}(0) = 0 \), and \( F_{n\ell}(r) = 0 \) at \( r = r_{\text{max}} \), we omit the first and last B-splines respectively. The coefficients \( c_{ni} \) of B-spline are determined by diagonalizing the atomic Hamiltonian \( H_0 \),
\[ < \phi_{n'\ell'\ell'} | H_0 | \phi_{n\ell m} > = \varepsilon_{n'\ell'\ell'} \delta_{nn'} \delta_{\ell\ell'} \delta_{mm'}. \]  (9)

The eigen energies obtained for lowest eight eigen states are found to be closer to the exact ones.

By substituting equation (4) into the Schrödinger equation (1) we have coupled equations with respect to the expansion coefficients \( a_{n'\ell'\ell'}(t) \),
\[ i \frac{d}{dt} a_{n'\ell'\ell'}(t) = \sum_{n\ell m} \epsilon_r \varepsilon_{n'\ell'\ell'} - \varepsilon_{n\ell m} | V_{\text{int}} | \phi_{n\ell m} > a_{n\ell m}(t). \]  (10)

The above coupled equations are solved with the initial condition \( a_{n\ell m}(b, -\infty) = \delta_{n'\ell'\ell', 1s} \).

The sum of the probabilities \( P_{n\ell m}(b) = |a_{n\ell m}(b)|^2 \) over eigen states with positive energies gives the ionization probability for a particular impact parameter. The ionization cross section can be obtained as
\[ \sigma = 2\pi \int_{0}^{\infty} P_{n\ell m}(b)bdb. \]  (11)
3. Results and Discussions

We solved the Schrodinger equation for $\bar{p}$ colliding with hydrogen and hydrogenic ions. Calculations are performed with 45 radial functions obtained from 8th order B-splines defined in the interval 0 to $r_{max}=200$ a.u. The maximum orbital angular momentum $l_{max}$ used in the calculation is 8. Since a single centred expansion calculation requires the retention of much higher values of angular momentum for producing well converged results. By taking all the degeneracies for magnetic quantum number $m$, we solved the coupled differential equation (10) with $2025(m \geq 0)$ number of basis sets. We integrated equation (10) in the interval $vt = -30 \ a.u.$ to $vt = 50 \ a.u.$ we considered the motion of the projectile along z axis and x-z is the collision plane.

Figure 1 displays the total cross sections for $\bar{p}$-H ionization. For comparison we also displayed the results obtained from other theoretical approaches.

![Figure 1. Total ionization cross sections of H under $\bar{p}$ impact](image)

The present calculated ionization cross sections are found to be in good agreement with the results of Tong et al (2001) throughout the energy range considered. This calculation has been carried out with straight line trajectory. It may be mentioned
that these authors also performed a calculation using curved trajectory which is not presented here. The results of one center Hilbert space calculation Hall et al are found to be a little higher than the present calculated values in the energy range between 20-100 kev impact energies. However, the once center calculation of Igarshi et al which uses Sturmian basis is found to be in resonably good agreement with the present values. The results of Sakimoto (2000) who used Laguerre meshes and the TDSE results of Wells et al are a little higher than our calculated values. Wells et al used a numerical solution of three dimensional Cartesian co-ordinate grids. The results of direct solution is always larger than the other calculated values. They mentioned that consideration of only $n \leq 3$ bound channels is insufficient and the estimated cross sections would overestimate. The calculation of Pons which makes use of the spherical Bessel functions to describe continuum channels are consistent with the present calculation. The recent calculation of Azuma et al who used the B-spline bases similar to the present one is found be in better agreement except around 0.1 keV impact energies. At this incident energy the present value slightly overestimates the calculation of Azuma et al.

![Figure 2](image-url)

**Figure 2.** Total ionization cross sections in $\bar{p}$ - H collisions, solid line : present results, closed circle : expt.data (Knudsen et al (1995))
In figure 2 we compare the present calculated results with available experimental measurements of Knudsen et al (1995). There is a good agreement between the present results and the experimental data over the whole energy range considered.

It clear from Figs. 1 that all the results for total ionization calculated using different approaches show reasonably good agreement in both qualitative and quantitative measures. All the theoretical values including the present one (Fig. 2) are in good agreement with the experiment of Knudsen et al. It will be interesting if the experiment measures the cross section data down to 1 keV energy range. We hope these will be available soon. In figure 3 we plotted $bP(b)$ as a function of impact parameter $b$ for several incident energies. It may be observed from the figure that the probability for high impact energy shows long tail and it dissapears as the collision energy decreases. The pack values also shifts to the lower impact parameter as the collision energy decreases.

In Fig. 4 we display the results of our single center B-spline basis set calculation for total ionzation cross section of He$^+$ by $\bar{p}$ impact for a wide energy range from 1 keV.
ionization of atomic hydrogen and He$^+$ by slow antiproton to 500 keV.

![Graph showing total ionization cross section of He$^+(1s)$](image)

**Figure 4.** Total ionization cross section of He$^+(1s)$, solid line: present results, solid circle: LTDSE (Schultz et al 1997), dashed line: SCE (Ford et al. Private communication), long dashed line: BGM (Kirchner et al 1999).

For comparison we also show in the figure, the results obtained by Lattice Schrodinger-equation approach (LTDSE) (Schultz et al 1997) and Single center results (Ford et al (private communication), Wherman et al (1996) and references therein). Also included in the figure are the results of Kirchner et al who used Basis Generator Method (BGM). This method deals with the construction of a basis that dynamically adapts to the collision process considered in order to follow the propagation and to cover the one dimensional subspace defined by the solution of the time dependent Schrodinger equation (TDSE). It may be seen in the figure that the present results are found to be in good agreement with the calculation of Ford et al who employed a single centred Hilbert basis set. However, both LTDSE and BGM results slightly overestimate the present cross sections. It has been mentioned in the paper of Schultz et al that this overestimation in comparison to the results of Ford et al is about 10%. They reported that this may due to the fact that it is likely that the excitation of He$^+$ to higher $n$
ionization of atomic hydrogen and He\(^+\) by slow antiproton

values probably \( n \geq 4 \), which has been incorrectly treated as ionization in LTDSE grid. They finally concluded that the treatment of excitation to \( n \geq 4 \) would be important in their method. Additionally other factors such as grid spacing would also needs to be carefully examined in order to calculate the ionization result beyond an accuracy of 10%.

\begin{figure}[h]
\centering
\includegraphics[width=\linewidth]{figure5.png}
\caption{Ionization probabilities in \( \bar{p} - \text{He}^+(1s) \) collisions as a function of impact parameter \( b \) at various incident energies}
\end{figure}

To support the present calculation, we displayed in Fig. 5 the variation of ionization probability with the impact parameter for various collision energies. It may be noted that \( b \ P(b) \) as function of \( b \) shows long tail for higher impact energies which is well experienced in case of 500 keV impact energies. However, for all collision energies peaks around \( b = 0.3 \) a.u. are observed. We also derived the dynamic ionization probability at this impact parameter (0.3 a.u.) when the two nuclei are separated from each other at some distance.

This is shown in Fig. 6. It is clear from the figure that the ionization probabilities saturate around \( z(\nu t) = 10 \) a.u. for all impact energies except 500 keV where the saturation starts early around \( z(\nu t) = 3a.u. \). The probability shows a rapid growth
between -3 and 3 a.u. and then saturation starts. Therefore we allowed sufficient time for the probability to become completely stable. The same type of situation has been shown by Tong et al (2001) who used curved trajectory for \( \bar{p} - H \) ionization. They have reported that for high collision energies (above 1 keV) the probability saturates \( z(vt) \) above 10 a.u. with a rapid increase from \( Z(vt) = -5 \) a.u.. For collision velocities (below 1 keV), they found a slow increase of the probability. This time delay can be termed as post-collisional interaction. Pons (2000) indicated that that due to slow antiproton motion the projectile pushes away the ejected electron even when the projectile is going farther from the target. Afterall in the present case Fig. 5 helps for a convergence check.

It may be worth to mention that in the case of \( \bar{p} - H \) ionization, where in the limit of small internuclear distance, the electron experiences a dipole like potential bound by two nuclei (Krstic et al 1996) and there exists a critical value of the dipole strength below which no bound state can be supported. It corresponds to the internuclear distance known as Fermi-Teller radius (Fermi and Teller 1947) at which the eigen energies of the
ionization of atomic hydrogen and He$^+$ by slow antiproton

ground state merge with the continuum. However, in case of an asymmetric dipole as in $\bar{p}$ - He$^+$ case, Krstic et al reported that the electronic eigen states donot merge with the continuum and hence the ionization cross sections are expected to show an exponential decrease for small collision velocities. These situations are clearly evident in Fig. 1 and Fig. 2.

4. Conclusions

The results obtained for $\bar{p}$ - H are found to be in good agreement with the other calculated values as well as the available experimental data. However, the experimental results are still awaited in low energy range. For the case of He$^+$ target, all the theoretical calculations including the present one show good agreement within a few percent of accuracy. Specifically the present results and the results of Ford show a good convergency. Our B-spline basis results confirms the single center Hilbert space calculation of Ford. There is no measured values for this system. It would be interesting to have more calculations for slow $\bar{p}$ projectile colliding with He$^+$.

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