A new time-dependent scattering theory and its application to the capture of antiprotons by atoms

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\textbf{Abstract.} We presented a theoretical method to study the capture of the antiprotons by atoms solving a Chew-Goldberger-type integral equation directly. The scattering boundary conditions are automatically satisfied by adiabatically switching on the interaction between the antiprotons and targets. Hence the outgoing wave function is obtained without the tedious procedure of adjusting the total wave function in the asymptotic region. All the dynamical information can be derived from the scattering wave function obtained on pseudo-spectral grids numerically. Using this method, we obtained the state-specified capture cross sections when antiprotons collide with helium atoms. Differing from the capture processes of antiprotons by hydrogen atoms, the anomalous bumpy structures are revealed in the angular momentum dependent capture cross sections by helium atoms. Further analysis shows that the bumps arise from the partial channel closing due to the removal of the energy degeneracy in the antiprotonic helium atoms.

\section{1. Introduction}
Coulomb three-body rearrangement collision is a prototype of general ion-atom collisions and electron-atom collisions. For heavy negative charged particles captured by atoms, the number of capture channels increases dramatically due to the huge mass difference between electron and negative charged particles. Thus, the computational time required for the nonperturbative approaches, e.g., the close-coupling method, inevitably increases dramatically as discussed by Esry and Sadeghpour \cite{1}. It is very difficult to solve the scattering equations without reducing the antiproton mass artificially. Protonium formation cross sections were calculated by scaling down the proton and antiproton masses to 20 a.u. Hesse \textit{et al.} \cite{2} used a diabatization technique to calculate the protonium formation but they were also obliged to use scaled proton and antiproton masses of 100 a.u. Their formation cross sections are peaked at $n = 7$, which is much lower than the estimated value of $n = 30$ for the protonium with the real mass, 1836 a.u. Cohen \cite{3} calculated the protonium formation cross section by the classical trajectory Monte Carlo (CTMC) method. The applicability of the classical mechanics at such low energies is not clear, especially for the motion of electron. Besides ambiguity occurs in extracting the discrete quantum numbers $n$ and $\ell$ from the classical continuous quantities.
Sakimoto [4] studied the formation process using a time-dependent wavepacket method but he did not obtain the state-specified formation cross sections due to the numerical difficulty. Ovchinnikov and Macek [5] applied the advanced adiabatic approach to calculate the n-dependent formation cross sections. Although their sophisticated method may be accurate qualitatively for the relevant process, it is not easy to estimate the quantitative reliability for the minute information such as the \((n, \ell)\)-distribution. Yamanaka and Ichimura [6] studied the protonium formation by solving Faddeev equations involved the ejected electron in the s-wave states only. To the best of our knowledge, reliable state-specified formation cross sections have not been obtained yet from nonperturbative quantal calculations apart from our recent works [7, 8, 9].

As mentioned above, the traditional coupled-channel method for the time-independent differential Schrödinger equation is not practically applicable to the process. To solve the problem differently, we started from the Chew-Goldberger integral equation of the scattering equation. The advantage of this method is that we transfer the complicated boundary conditions into a simple initial condition and convert the time-independent scattering theory into the time-dependent scattering theory. The theoretical details will be presented in the following section, followed by the applications of the theory to the captures of antiprotons by helium atoms.

2. Theoretical Method

2.1. General time-dependent formalism

The time-independent Schrödinger equation of a Coulomb three-body system in the center-of-mass frame is written as (atomic units \(\hbar = m_e = e = 1\) are used hereafter unless otherwise stated)

\[
H\Psi(t) = E\Psi(t),
\]

with

\[
H = -\frac{1}{2\mu_e} \nabla_r^2 - \frac{1}{2\mu_p} \nabla_R^2 + V_{n,e}(r) + V_{n,p}(R) + V_{\bar{p},e}(r,R).
\]

Here \(E = E_c + E_{1s}\) is the total energy of the collision system in the center-of-mass frame with \(E_c\) the incident energy of the projectile and \(E_{1s}\), the ground state energy of the target atom. \(r\) and \(R\) are respectively the distances from the nucleus to the electron and from the center-of-mass of the atom to the projectile. \(V_{n,e}(r), V_{n,p}(R),\) and \(V_{\bar{p},e}(r,R)\) are the interactions of the nucleus and the electron, the nucleus and the antiproton, and the electron and the antiproton, respectively. \(\mu_e\) is the reduced mass of the nucleus and the electron and \(\mu_p = M_p(m_e + m_n)/(M_n + m_e + M_p)\). \(M_n, m_e,\) and \(M_p\) are the masses of nucleus, electron and antiproton, respectively. The solutions of Eq. (1) satisfying proper boundary conditions can be expressed as an integral expression;

\[
\Psi(t) = \Psi_i - i\int_{-\infty}^{t} e^{-i(H-E)(t-t')} f(t') V_i \Psi_i dt'.
\]

Here, \(V_i\) is the interaction between the initial state and the complete state. The time-dependent wave function \(\Psi(t)\) goes back to the initial state as \(t \to -\infty\), and it also satisfies Eq. (1) at \(t = 0\) if \(f(-\infty) = 0,\) \(f(0) = 1\) and \(f(t)\) switches on adiabatically \([10]\), i.e., \(\frac{df}{dt}(t) \to 0\). A choice of \(f(t) = \exp(-\eta|t|)\) gives Chew-Goldberger formal solution at \(t = 0\) as

\[
\Psi^+ = \Psi_i + \frac{1}{E - H + i\eta} V_i \Psi_i,
\]

where \(\eta\) is a positive infinitesimal number. We calculated the time-dependent wavefunction by integrating Eq. (3) instead of solving Eq. (1) or Eq. (4). \(f(t)\) can be any function so long as it is switched on adiabatically. For instance, \(f(t) = \exp(-t^2/\tau^2)\) can be used for \(\tau \to \infty\). Once obtaining \(\Psi^+(t = 0)\) by propagating Eq. (3), we can derive all the dynamical information of the collision system.
2.2. Numerical procedures
Coulomb three-body systems cover a variety of physical processes. The characteristic of each system depends strongly on the combination of the masses and the charges of the constituting particles. We focused on dealing with heavy negatively-charged particles, antiprotons, colliding with helium atoms as an example to show how to propagate Eq. (3) effectively and accurately. The initial wave function $\Psi_i$ of the system is the product of the ground state wave function of the target atom and the wave function of the projectile, which is expressed as

$$\Psi_i(r, R) = \psi_{1s}(r) \psi_e(k_0, R).$$ (5)

Here $k_0$ is the initial momentum of the projectile in the center-of-mass frame, $\psi_{1s}(r)$ the ground state wave function of the Hamiltonian $H(r) = -\frac{1}{2\mu_e} \nabla_r^2 + V_{n,e}(r)$ and $\psi_e(k_0, R)$ the wave function of the Hamiltonian $H = -\frac{1}{2\mu_p} \nabla_R^2 + V_{n,p}(R) - \frac{1}{R}$ with the incoming wave boundary condition. The Hamiltonian of the initial channel and the corresponding interaction are

$$H_i = -\frac{1}{2\mu_e} \nabla_r^2 + V_{n,e}(r) - \frac{1}{2\mu_p} \nabla_R^2 + V_{n,p}(R) + \frac{1}{R},$$ (6)

$$V_i = V_{p,e}(r, R) - \frac{1}{R}.$$ (7)

Because the total angular momentum $L$, its component $M$ onto the incident beam direction, and the parity are good quantum numbers, we expand the time-dependent wave function as

$$\Psi(t) = \sum_{LM} \Psi_{LM}(r, R, t) = \sum_{LM} \sum_{\alpha} F^{\alpha}(r, R, t) \Omega_{LM}^{\alpha}(l_e, l),$$ (8)

with

$$\Omega_{LM}^{\alpha} = \sum_{m_e, m} <l_m|m_eLM > Y_{l,m_e}(\hat{r}) Y_{l_m}(\hat{R}).$$ (9)

Here $\alpha$ is a index to represent the angular momentum ($l_e$) of the electron, the angular momentum ($l$) of the antiproton, and the parity collectively. Each $\Psi_{LM}(r, R, t)$ can be propagated independently. The radial Hamiltonian for a given $LM$ is written as

$$< \Omega_{LM}^{\alpha} | H | \Omega_{LM}^{\alpha'} > = \left( -\frac{1}{2\mu_e} \frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{2\mu_e r^2} + V_{n,e}(r) \right) \delta_{\alpha,\alpha'} + \left( -\frac{1}{2\mu_p} \frac{\partial^2}{\partial r^2} + \frac{l_e(l_e+1)}{2\mu_p r^2} + V_{n,p}(R) \right) \delta_{\alpha,\alpha'} + < \Omega_{LM}^{\alpha} | V_{p,e}(r, R) | \Omega_{LM}^{\alpha'} >$$

$$= H^{\alpha}(r) + H^{\alpha}(r) + \mathbf{V}^{\alpha,\alpha'}(r, R).$$ (10)

After the partition, the time propagation from time $t$ to $t + \Delta t$ was performed by the split-operator method in the energy representation [11, 12] as

$$U(t + \Delta t, t) = e^{-iV(r,R)\Delta t/2} e^{-iH(R)\Delta t} e^{-iH(r)\Delta t} e^{-iV(r,R)\Delta t/2} + O(\Delta t^3).$$

We first propagated the wave function a half-time step in $V(r, R)$, and then a full-time step in $H(r)$ and $H(R)$, and finally another half-time step in $V(r, R)$. The advantage of this time-propagation scheme is that each operator is diagonal in the other two dimensions. $V(r, R)$ couples only different channels $\alpha \neq \alpha'$ and $H(R)$ and $H(r)$ are, on the other hand, diagonal for $(\alpha, \alpha')$. These characters make the time propagation computationally efficient.
For three-body rearrangement collisions, we have to deal with continuum wave functions. In the direct integration method on grid points, the coordinate space is confined in a finite box. We have to filter out the outgoing waves at the boundary in order to eliminate the unphysical reflection. For this purpose, we added an optical potential near the boundary to absorb the outgoing flux. The optical potential we used is of the form of

\[ V_{\text{opt}}(\epsilon, r) = \begin{cases} 
0 & \text{for } r < r_c \\
-iV_0 \left( \frac{r-r_c}{r_{\text{max}}-r_c} \right) & \text{for } r \geq r_c 
\end{cases} \]

with \( V_0 \) in the form suggested in Ref. [13]. Here \( \epsilon \) is the energy of the basis wave function and \( r_{\text{max}} \) and \( r_c \) are the position of the boundary in the radial direction and the start of the filter, respectively. \( \mu \) is the reduced mass associated with coordinate \( r \). The optical potential added to Hamiltonian \( H(r) \) is

\[ V_{\text{opt}}(r) = \sum_i V_{\text{opt}}(\epsilon_i, r) |\psi_i> <\psi_i| \quad \text{for } \epsilon_i \geq 0, \]

where \( \{\epsilon_i\} \) and \( \{\psi_i\} \) are the eigen energies and eigen wave functions of \( H(r) \). \( V_{\text{opt}}(r) \) depends on the grid structure but it does not depend on the collision energy. It is a universal optical potential which can be used to absorb the ejected electron in a broad energy range. Similarly we add an optical potential to \( H(R) \). After a time propagation from \( t = -\infty \) to \( t = 0 \), in the interaction region, we obtain the scattering wave function \( \Psi^+(t=0) \), which satisfies the proper boundary conditions. The final wave function corresponding to the capture to the state of a principal quantum number \( n \) and an angular momentum \( l \) is expressed as

\[ \Psi^\alpha_j = j_l(k_{nl}r)\psi_{nl}(R)\Omega^\alpha_{LM} \]

where \( k_{nl} \) is the ejected electron momentum associated with the formation of an exotic atom in the \( nl \) state. The \( T \)-matrix element is given by

\[ T^\alpha_{nl} = <\Psi^\alpha_j|V_f|\Psi^+_{LM}> \]

and the state specified capture cross section is readily obtained as

\[ \sigma_{nl}(L) = \frac{4\mu_{\bar{p}} \mu_e k_{nl}}{k_0} \sum_\alpha |T^\alpha_{nl}|^2. \]

### 3. Results and Discussion

Based on the above theoretical method, we can investigate the dynamical processes involved in a Coulomb three-body problem or many-body problem which can be reduced to a three-body problem approximately. Following, we will present our studies on the antiproton captured by helium atoms. Frozen one of the two electrons in the collision system, the electron-core interaction \( V_{n,e}(r) \) is approximated as \( V_{e,eff}(r) \), a six-parameter model potential [14] and the antiproton-core interaction \( V_{n,\bar{p}}(R) \) is approximated as \( U(R) \), the effective potential of the antiproton moving in the combined field of the helium nucleus and the passive electron in the ground state and it can be calculated from the following equation adiabatically

\[ H_n \Psi(r_2; R) = U(R)\Psi(r_2; R). \]

The electron-antiproton interaction is a pure Coulomb interaction. With the above approximations, we solve the time-dependent Schrödinger equation (Eq. (7)) as we did for antiproton captured by hydrogen atoms and obtain the state-specified capture cross-sections as
shown in Fig. 1. We also plot the state-specified capture cross-sections by hydrogen atoms for comparison. For hydrogen atoms, the capture cross-section changes smoothly as a function of the \((n, \ell)\). While for helium atoms, the capture cross-section peaks at higher \(n\) for lower \(\ell\). At the same incident energy, the antiproton is captured to a higher \(n\) states for hydrogen atoms than that of helium atoms. This can be understood since the effective charge of helium atoms is larger than that of hydrogen atoms and the antiproton can only be captured to the lower \(n\) states due to the conservation of energy. Although the state-specified cross sections contain all the necessary information to analyze the experiment, it is difficult to see the details from the 2-dimensional color plot. Now we sum over all \(n\) for a given \(\ell\) to study the \(\ell\)-dependent capture cross-section as shown on the left panel in Fig. 2.

For the capture by hydrogen atoms, the capture cross sections increase smoothly as \(\ell\) increases, reach a peak at \(\ell = 35\) and then drop quickly as \(\ell\) increases further. For the capture by helium atoms, the capture cross sections first increase in an irregular manner, reach the maximum at \(\ell = 38\), and then, drop sharply. This global feature is similar to the capture of antiprotons by hydrogen atoms. Unlike the hydrogen case, however, the present cross sections show the anomalous bumpy structures. It is notable that the present calculations are more difficult than those of the hydrogen case due to the larger reduced mass \(\mu_p\) and the larger effective charge of helium. To check the numerical accuracy, the simulation conditions, such as the number of grids, the size of the space surrounding the whole system, and so on, have been varied. As a result, it is convinced that the anomalies manifested on the left panel of Fig. 2 are insensitive to the changes of these parameters. Thus, the anomalies are ascribable to a certain
physics, not due to the numerical inaccuracy.

Although the capture process of the antiprotons by hydrogen atoms and helium atoms are similar within the present approximation, the energy structures of protonium ($\bar{p}p$) and antiprotonic helium ($\bar{p}\text{He}^+$) are different. Replacing the Coulomb potential in the former by the effective potential in the latter, the energy degeneracy assigned by $n$ and $\ell$ is removed, where $n$ and $\ell$ are the principle and angular momentum quantum numbers, respectively. As shown on the right panel of Fig. 2, the energy curves for a given $n$ and different $\ell$ cross over with the total energy (dashed straight line). The cross over positions are in good agreement with the dip positions in the $\ell$-dependent capture cross sections. Let us focus on $n = 47$ as an example to show the origin of the dips. With the 10 eV incident energy, the antiprotons can be captured to $n = 47$ with $\ell \leq 11$ due to the energy conservation. This means that this channel is opened for the capture to $\ell \leq 11$ states and is closed for the capture to $\ell \geq 12$ states. This fact would allow us to speculate that the manifestation of the anomaly around $\ell = 12$ is attributed to the channel closing of the states with $\ell \geq 12$. Here, the channel closing means that for a given $n$ the capture process is forbidden when the $\ell$ is larger than a critical value. In a similar way, it is shown that the next dip corresponds to the closing of channel $n = 46$ at $\ell = 23$, and so on. In general, the partial inelastic scattering cross sections exhibit cusps when the incident energies cross a new threshold since the cross sections differ significantly for the energies below and above the threshold. Here we found cusps from a different aspect, i.e., the cross sections as a function of the $\ell$ for a given incident energy and $n$. The similar phenomena are also observed at other incident energies with the change of the dip positions and hence this anomaly is considered as a general phenomenon.

To summarize, we presented a new time-dependent scattering theory, which can be used to study general Coulomb three-body rearrangement processes. The key procedure is that we transferred the very complicated boundary conditions into a simple initial condition. Using this method, we obtained the state-specified capture cross sections when antiprotons collide with hydrogen atoms or helium atoms. Differing from the capture processes of antiprotons by hydrogen atoms, the anomalous bumpy structures are revealed in the total angular momentum dependent capture cross sections by helium. Further analysis shows that the bumps arise from the partial channel closing due to the removal of the energy degeneracy in the antiprotonic helium atom.

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