Scaling relation in the collision of hydrogenlike ions with antiprotons

Xiao-Min Tong,[1,*] Tsutomu Watanabe[1,2] Daiji Kato,[1] and Shunsuke Ohtani[1,2]
[1]*"Cold Trapped Ions" Project, ICORP, Japan Science and Technology Corporation (JST), Axis Chofu Building 3F, 1-40-2 Fuda Chofu, Tokyo 182-0024, Japan*
[2]*University of Electro-Communications, Chofu, Tokyo 182-0021, Japan*
(Received 10 June 2001; revised manuscript received 17 May 2002; published 19 September 2002)

The impact excitation and ionization of hydrogen (H)-like ions by antiprotons are studied by solving the time-dependent Schrödinger equation with a time-dependent generalized pseudospectral method in a wide scaled impact energy region (1 to 1000 keV). The validity region of the scaling relation is investigated by comparing the time-dependent calculations with the first Born approximation results. The numerical error and the validity region of the time-dependent generalized pseudospectral method have been explored. Based on the present study, we conclude that (i) the scaling relation of the ionization and excitation cross sections is valid for high-Z H-like ions or in the high-impact-energy regime for low-Z H-like ions; (ii) for given H-like ions, the scaling relation works better for the impact excitation to the dipole allowed transition than for the impact excitation to the dipole forbidden transition; and (iii) the time-dependent generalized pseudospectral method is not valid in a very weak perturbation system, which can be fairly studied by the time-independent methods. We also discuss the physical originations of the numerical observations.

DOI: 10.1103/PhysRevA.66.032708 PACS number(s): 34.50.Fa, 34.10.+x, 25.43.+t

I. INTRODUCTION

The collision between hydrogen atoms and antiprotons ($\bar{p}$) is one of the simplest and most fundamental processes in atom-ion collision physics. There are many theoretical works [1–10] on this simple system. An experimental research using slow antiprotons is prepared under the project of atomic spectroscopy and collisions using slow antiprotons (ASACUSA) [11] at the Antiproton Decelerator (AD) in CERN, which stimulates more recent theoretical works [12–16]. In the first Born approximation, the impact excitation and ionization cross sections of hydrogen (H)-like ions by antiprotons are the same as that of H-like ions by protons. The cross sections have a scaling behavior for being in the first Born approximation. In recent theoretical studies [4,9,10,17] it is found that the ionization cross section does not fall off in the low-energy regime for the collision of H atoms by antiprotons. The ionization cross sections are different for protons and antiprotons collision with H atoms at the low-energy regime. Thus, we can see that the first Born approximation is not valid in the low-energy regime for collision between H atoms and antiprotons. Now the question is whether or not the first Born approximation is valid in the low-energy regime for collision between the H-like ions and antiprotons. To our acknowledge, there are a few theoretical studies on the collision of H-like ions with antiprotons [9,18] and there is no experimental data so far. Of course, from the experimental point of view, such an experiment is extremely difficult due to the low ion density and small cross sections. But from a theoretical point of view, the collision between H-like ions and antiprotons provides a system to study (i) the validity of the scaling relation, and (ii) comparison between the time-dependent and time-independent methods. Meanwhile, the ionization cross sections of H-like ions can be used to study the multi-electron ionization process in the independent event model [19] when the sequential ionization is dominant. Here we calculate the impact ionization and excitation cross sections of H-like ions by antiprotons using a time-dependent generalized pseudospectral (TDGPS) method combined with the split-operator method in the energy representation [20]. Such a TDGPS method has been successfully applied to study the high-order harmonic generation in the intense laser field [21], high-resolution spectroscopy of the Rydberg atom in the crossed electric and magnetic fields [22], and the collisions of H atoms with protons [23,24] or antiprotons [17]. The purposes of the present study are threefold: (i) the validity of the scaling relation; (ii) the comparison between the time-dependent and time-independent methods; and (iii) the numerical error analysis in the present TDGPS method.

We will present our theoretical method in Sec. II, which is emphasized on the scaling behavior in the working equations and error analysis in the second-order split-operator method. The calculated results and a discussion will be presented in Sec. III, followed by a summary in Sec. IV.

II. THEORETICAL METHOD

The impact excitation and ionization cross sections of H-like ions by antiprotons can be studied by a time-dependent method as well as by a time-independent method (perturbation method), like the first-order Born approximation. Following, we will introduce the two methods.

A. Time-dependent method

The collision between H-like ions and antiprotons can be studied by the impact parameter method, in which the relative motion of the antiproton with respect to the atomic nucleus is described by classical mechanics, and the time-

*Present address: Physics Department, Kansas State University, Manhattan, Kansas 66506. Email address: xmtong@phys.ksu.edu

evolution of the electron motion is described by quantum mechanics. The time-dependent electron wave function of the H-like ions can be described by the following time-dependent Schrödinger equation as (atomic units with $\hbar = m = e = 1$ are used throughout unless explicitly stated otherwise)

$$i\frac{\partial}{\partial \tilde{t}}\psi(\tilde{\mathbf{r}},\tilde{t}) = \tilde{H}(\tilde{t})\psi(\tilde{\mathbf{r}},\tilde{t}) \tag{1}$$

with

$$\tilde{H} = -\frac{\tilde{\nabla}^2}{2} - \frac{Z}{\tilde{r}} + \frac{1}{|\tilde{\mathbf{R}}-\tilde{\mathbf{r}}|}, \tag{2}$$

$$\mu\ddot{\tilde{\mathbf{R}}} = -\nabla\tilde{V}(\tilde{\mathbf{R}}), \tag{3}$$

$$\tilde{V}(\tilde{\mathbf{R}}) = -\frac{Z}{\tilde{R}} + \int \frac{\psi^*(\tilde{\mathbf{r}},\tilde{t})\psi(\tilde{\mathbf{r}},\tilde{t})}{|\tilde{\mathbf{R}}-\tilde{\mathbf{r}}|}d\tilde{\mathbf{r}}. \tag{4}$$

Here Z is the target nuclear charge of the H-like ions and μ is the reduced mass of the H-like ion and the antiproton. We suppose that $\bar{p}$ is approaching the target (an H-like ion), which is rested at the origin, along the z direction with a velocity v, and the impact parameter b along the x direction. We also assume that the relative motion of the incident $\bar{p}$ with respect to the target nucleus follows a classical trajectory, from Eq. (3). To investigate the scaling relation of the impact excitation and ionization cross sections in the collision of H-like ions by antiprotons, we make the following transformations:

$$\tilde{\mathbf{r}} = \mathbf{r}/Z \quad \tilde{\mathbf{R}} = \mathbf{R}/Z$$

$$\tilde{t} = \mathbf{t}/Z^2 \quad \tilde{H} = Z^2 H. \tag{5}$$

Now, we rewrite Eqs. (1)–(4) as

$$i\frac{\partial}{\partial t}\psi(\mathbf{r},t) = H(t)\psi(\mathbf{r},t) \tag{6}$$

with

$$H = -\frac{\nabla^2}{2} - \frac{1}{r} + \frac{1}{Z|\mathbf{R}-\mathbf{r}|}, \tag{7}$$

$$\mu\ddot{\mathbf{R}} = -\nabla V(\mathbf{R}), \tag{8}$$

$$V(\mathbf{R}) = -\frac{1}{R} + \int \frac{\psi^*(\mathbf{r},t)\psi(\mathbf{r},t)}{Z|\mathbf{R}-\mathbf{r}|}d\mathbf{r}. \tag{9}$$

Equation (6) can be solved by the second-order split-operator method with a generalized pseudospectral grid in the energy representation [20,23,24] as

$$\psi(t+\Delta t) = e^{-iH_0\Delta t/2}e^{-iV(t)\Delta t}e^{-iH_0\Delta t/2}\psi(t) + O(\Delta t^3)\psi(t) \tag{10}$$

with

$$H_0 = -\frac{\nabla^2}{2} - \frac{1}{r}, \tag{11}$$

$$V(t) = \frac{1}{Z|\mathbf{R}-\mathbf{r}|}, \tag{12}$$

$$O(\Delta t^3) = \frac{i}{24}\{[V(t),H_0],H_0+2V(t)\}\Delta t^3. \tag{13}$$

To propagate the wave function in Eq. (10), we use spherical coordinates, and the radial part is discretized by the generalized pseudospectral method [25]. The detailed numerical procedure can be found in Refs. [20,23,24]. With this impact parameter method, we can propagate the wave function from $t = 0 \rightarrow T$ with the projectile along the z direction starting from z_0. The initial wave function is located in the target ground state. When the projectile passes through the target and far from the target, we obtain the excitation or ionization probability as

$$P(T,b) = |<\psi(T)|\psi_f>|^2, \tag{14}$$

where ψ_f is the time-independent excited or continuum state wave function centered at the target H-like ions. The corresponding cross sections in the scaled coordinates can be obtained as

$$\sigma = 2\pi\int P(T,b)bdb. \tag{15}$$

The cross section for a given H-like ion can be obtained as

$$\tilde{\sigma} = \frac{\sigma}{Z^2}. \tag{16}$$

Since the interaction between the target electron and the antiproton is scaled as $1/Z$ in Eq. (12), the cross section in Eq. (15) should be

$$\sigma \propto \frac{\sigma^H}{Z^2} \quad \text{or} \quad \tilde{\sigma} \propto \frac{\sigma^H}{Z^4} \tag{17}$$

with σ^H as the cross section for H atoms. For the convenience of later discussion, we define a scaled probability, scaled cross section, and scaled impact energy as

$$P_s(T,b) = Z^2 P(T,b), \tag{18}$$

$$\sigma_s = Z^4\tilde{\sigma}, \tag{19}$$

$$E_s = E/Z^2. \tag{20}$$

B. Time-independent method

In the first-order plane wave Born approximation, the impact excitation and ionization cross sections of H atoms by antiprotons can be written as

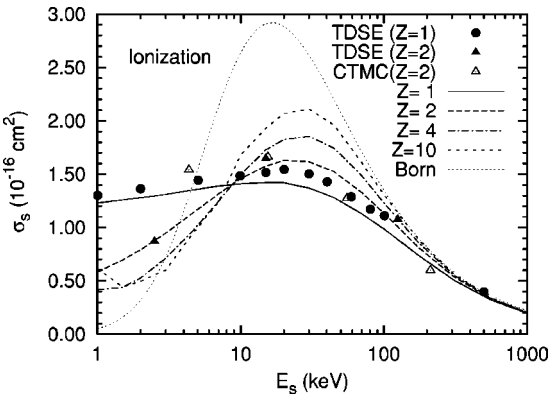

FIG. 1. The scaled impact ionization cross sections of the H-like ions by antiprotons together with other theoretical calculations. Filled circles are from Ref. [9], open triangles are from Ref. [10], and filled triangles are from Ref. [18].

$$\sigma = \begin{cases} \dfrac{8\pi}{v^2}\displaystyle\int_{q_{min}}^{q_{max}} F_{ij}(q)/q^3 dq & \text{excitation,} \\ \dfrac{8\pi}{v^2}\displaystyle\int\int_{q_{min}}^{q_{max}} F_{ij}(q)/q^3 dq d\epsilon & \text{ionization} \end{cases} \tag{21}$$

with

$$F_{ij}(q) = |\langle \psi_i | e^{-i\mathbf{qr}} | \psi_j \rangle|^2. \tag{22}$$

Here, ψ_i and ψ_j are the initial and final states of the H-like ions, q is the momentum transfer, v is the impact velocity, and q_{min} and q_{max} are the minimum and maximum momentum transfers for a given energy loss. For the H-like ions, the cross sections can be written as

$$\sigma(Z) = \sigma^H / Z^4. \tag{23}$$

The scaling relation, Eq. (23), is exact in the first Coulomb projected Born approximation.

III. RESULTS AND DISCUSSION

Based on the TDGPS method with the second-order split-operator method in the energy representation [20], we calculated the impact excitation and ionization cross sections of H-like ions ($Z=1,2,4,10$) by antiprotons. All the calculations were performed in a 4 PC Linux cluster with a Pentium III 400 MHz CPU. The numerical convergence has been checked in the same way as we did for the collision of H atoms by antiprotons [17]. For comparison, we also calculated the impact excitation and ionization cross sections by the first-order Born approximation. Since the Born approximation is valid in high-impact-energy, we expect that the time-dependent and Born results should agree with each other at the high-impact-energy regime.

Figure 1 shows the scaled impact ionization cross section of H-like ions (Z=1,2,4,10) by antiprotons calculated by the present time-dependent Schrödinger equation method as well as by the first Born approximation. For comparison, other theoretical results [9,10,18] of the impact ionization cross section of H-like ions by antiprotons are also presented in Fig. 1. For the first Born calculation, the scaled impact ionization cross section is independent from the target atomic number Z. As we expected, the scaled ionization cross sections are in good agreement with each other at a high-impact-energy regime (above a few 100 keV). As the scaled impact energy goes to the medium-energy regime (from 20 to a few 100 keV), the scaled impact ionization cross sections increase more rapidly for the high-Z H-like ions. The maximum scaled ionization cross section appears around 25 keV, at which the incident velocity is equal to the $1s$ electron velocity moving around the target nucleus. In this energy regime, although the scaled ionization cross sections of the high-Z ions are closer to the first Born results than those of the low-Z ions, significant discrepancies still exist, as shown in Fig. 1. The peak value of the first Born result is about 1.4 times the peak value of the scaled result for $Z=10$. As the scaled impact energy goes to the lower-energy regime (below 20 keV), the scaled ionization cross sections decrease very rapidly for the high-Z H-like ions. For H atoms, the ionization cross section decreases very slowly, as shown in Fig. 1, instead of the fast decrease predicted by the first Born approximation. The different behaviors of the ionization cross section for H-like ions by antiprotons at the lower-energy regime have been studied systematically by the theory of hidden crossing [9]. In this theory, at the united atom limit, the collision system of H atoms by antiprotons has no bound state. The initial ground state is pushed into a quasimolecular continuum state. This results in a finite ionization cross section at the lower-energy end. For high-Z ions, the initial ground state and the ground state of the united atom are close to each other. This results in the decrease of the ionization cross section as the impact energy decreases. Detailed explanation can be found at Ref. [9]. It is very interesting to compare our scaled ionization cross sections with other calculations. For H atoms, our results (solid line) are in good agreement with lattice time-dependent Schrödinger equation method (TSDE) (circles) results [10] within a few percentages over the whole-energy regimes. For He^+ ions, our results (dashed line) are in agreement with TDSE's results [18] (filled triangles) over the whole-energy regimes. The classical trajectory Monte Carlo (CTMC) calculation [9] (open triangles) is also in agreement with our results in the medium-energy region. In the lower-energy region, the scaled cross section of He^+ ions should be smaller than that of H atoms. But the CTMC result shows larger than that of the H atom. Therefore, we think the CTMC results at lower-energy are overestimated for the ionization cross sections. Our time-dependent calculation of the scaled ionization cross section for $Z=10$ shows some increasing, which is due to the numerical error we will discuss later.

Figure 2 shows the scaled $2s$ and $2p$ excitation cross sections of H-like ions by antiprotons. The TDSE results for He^+ from Ref. [18] (filled triangles) are in good agreement with the present calculation for both $2s$ and $2p$ excitation. The general features of the $2s$ excitation cross sections are quite similar to the ionization cross section. All the scaled $2s$ excitation cross sections are in good agreement at the high-

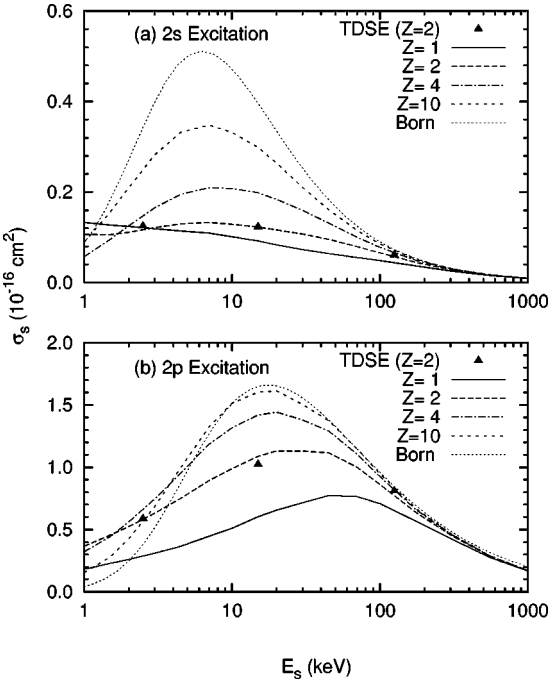

FIG. 2. The scaled excitation cross sections of the H-like ions by antiprotons to (a) $2s$ and (b) $2p$ states. Filled triangles are from Ref. [18].

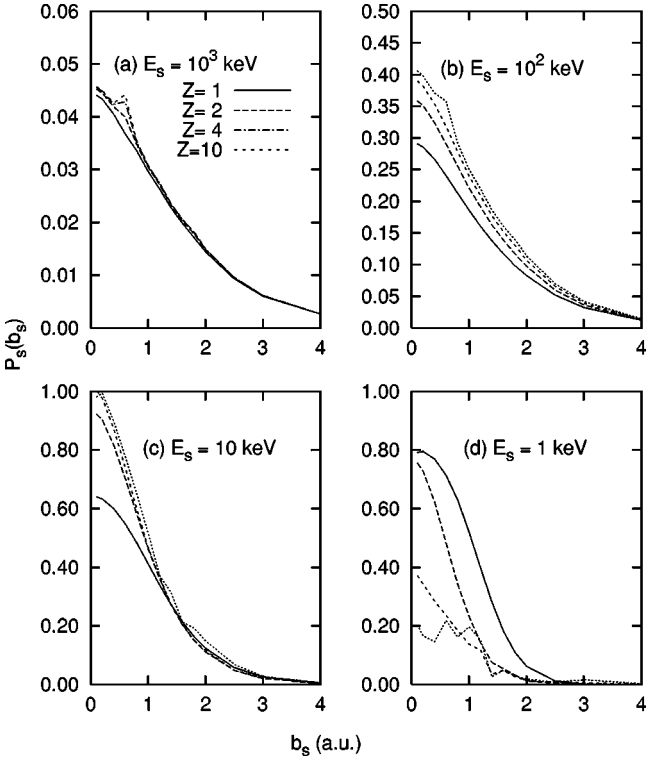

FIG. 3. The scaled ionization probabilities of H-like ions by antiprotons. The scaled impact energies are (a) 1000 keV, (b) 100 keV, (c) 10 keV, and (d) 1 keV, respectively.

energy regime. The peak value of the first Born result is about 1.6 times the peak value of the scaled result for $Z=10$. The difference is that the $2s$ excitation peaks are located in the lower-energy position, compared with the ionization cross sections. The $2s$ excitation cross section of H atoms increases monotonically as the impact energy decreases, as shown in Fig. 2(a), which was discussed by Krstic *et al.* [9].

Figure 2(b) shows the scaled $2p$ excitation cross sections of H-like ions by antiprotons. The general features of the $2p$ excitation cross sections are similar to the ionization, as well as the $2s$ excitation, as we vary Z from 1 to 10. A significant difference is that the first Born result is in good agreement with the scaled $2p$ excitation cross section for $Z=10$.

Based on the ionization and $2s$, $2p$ excitation shown in Figs. 1 and 2, we find that (i) the scaling relation of the ionization and the excitation cross sections is valid for high-Z H-like ions, or in the high-impact-energy regime, and (ii) for given H-like ions, the scaling relation works better for the impact excitation to dipole allowed transition than for the dipole forbidden transition. For the first observation, we see that the time-dependent Schrödinger equation and the perturbation methods should be the same when $\int V(t)dt$ in Eq. (10) is small. We can easily see that the scaling relation is valid for a short interaction time (high-impact energy) or a small interaction (high-Z case). In the Born approximation, generally speaking, the dipole allowed transition cross section is larger than the dipole forbidden transition cross section. This is due to the fact that the integration in Eq. (21) is dominated by the small q and the leading term in Eq. (22) is a dipole term. For simplicity, we decompose the $\int V(t)dt$ in Eq. (10) as a summation of monopole and dipole, i.e.,

$$\int V(t)dt = V_0 + V_1. \tag{24}$$

In the perturbation theory, we only consider the leading term in the expansion of $e^{-i\int V(t)dt}$, in which the scaling relation is valid. Now let us consider the next leading term, which will lead the invalidity of the scaling relation. For monopole, this term is proposed to be $V_0^2+V_1^2$. For dipole, this term is proposed to be $V^0 * V^1$. The relative effect for the monopole is much larger than that for the dipole since $V_1 > V_0$. Or, in other words, the scaling relation works better for the dominant transition. Indeed, we see the $2p$ excitation cross section is larger than that of $2s$ and the scaling relation works better for the $2p$ transition than for the $2s$ transition, as shown in Fig. 2.

In our calculation, originally, we thought that the time-dependent calculation for the scaled equation with high-Z should be easier and more reliable due to the relative weak interaction in Eq. (12). To our surprise, the most difficult case is $Z=10$, the largest Z in the present calculations. This forces us to check the origin of the numerical error and compare the advantage and disadvantage of the time-dependent Schrödinger equation method. In the split-operator time propagation, Eq. (10), the numerical error, Eq. (13), comes from three parts: (i) the finite number of the grid in the radial part; (ii) the finite number of the partial wave; and (iii) time step Δt. To obtain a reliable numerical result, we hope that $1-e^{-iH_0\Delta t/2}e^{-iV(t)\Delta t}e^{-iH_0\Delta t/2}$ is as large as possible and $O(\Delta t^3)$ in Eq. (10) is as small as possible. If $V(t) \ll H_0$, Eq.

(10) is vulnerable to the numerical error. We call the error related to the first term as E1 and the error related to the second term as E2. After each time step propagation in Eq. (10), if the change in the wave function $[\psi(t+\Delta t)-\psi(t)]$ is very small compared with the original wave function $\psi(t)$, which is the case for the weak interaction potential in Eq. (12), the numerical results will not be reliable anymore. If we increase the time step Δt, the change in the wave function increases, so as the error in Eq. (13). Thus, using the time-dependent Schrödinger equation method to study a weak perturbation system is not effective. In the time-independent perturbation methods, like the Born approximation, the initial state is factored out from the final states. Therefore, the time-independent perturbation theory is better for a weak perturbed system, like the high-Z H-like ions in the present calculations.

To support our above argument, the scaled ionization probability as a function of the impact parameter b is shown in Fig. 3 with four scaled impact energies: 1, 10, 100, and 1000 keV. We see that the scaled probability for low-Z ($Z=1,2$) ions is relatively smooth over the whole energy range (from 1 to 1000 keV). For high-Z ions (Z=4,10), the largest ionization probabilities ($1/Z^2$) are 1/16 and 1/100. For high-impact energy (1000 keV), the scaled ionization probability is about two orders too small. Therefore, the ionization probability of the high-Z ions at high-impact energy is vulnerable to the numerical error in the calculation. Since the interaction time is very short, the numerical error mainly comes from the E1 or grid structure, namely, when the impact antiproton is too close to the radial grid (Coulomb singularity). Such a numerical error [the bump in Fig. 3(a)] always exists, but plays an important role when the ionization probability is small. As the ionization probability increases at 100 keV impact energy, the contribution of such a numerical error is getting smaller, as shown in Fig. 3(b). The scaled probability goes too smoothly when it reaches maximum at 10 keV. Such a numerical error can be minimized by using a two-center grid structure or by choosing the grid structure more carefully in the numerical calculation. For the lowest energy in the present calculation, the ionization probability shows some oscillation for $Z=10$. Since the time step is relatively large in the lower-energy region, this part of the error comes from the E2 term, which is very difficult to be suppressed. Anyway, if the perturbed potential $V(t)$ is very weak, namely, $V(t)$ is in the numerical roundoff region comparing with H_0, the present time-dependent Schrödinger equation totally breaks down. The time-independent method, namely, the first Born approximation, should be used in this regime.

IV. SUMMARY

Based on the TDGPS method and the time-independent method (first Born approximation), we have studied the impact ionization and excitation of H-like ions impact by antiprotons. By comparing the scaled cross sections calculated by the time-dependent and time-independent methods, we found that (i) the scaling relation is valid in the high-impact-energy regime, which is already well known; (ii) the scaling relation is also valid for the high-Z H-like ions collision with antiprotons in the lower scaled impact energy regime; and (iii) the scaling relation works better for the dipole allowed transitions than for the dipole forbidden transitions for given ions. Meanwhile, we also found that the TDGPS method does not work well in a very weak perturbation system. Fortunately, such systems can be fairly studied by the time-independent perturbation method.

[1] D.R. Bates and G. Griffing, Proc. Phys. Soc., London, Sect. A **66**, 961 (1953).
[2] M.H. Martir, A.L. Ford, J.F. Reading, and R.L. Becker, J. Phys. B **15**, 1729 (1982).
[3] J. Cohen, Phys. Rev. A **36**, 2024 (1987).
[4] D.R. Schultz, Phys. Rev. A **40**, 2330 (1989).
[5] P.D. Fainstein, V.H. Ponce, and R.D. Rivarola, J. Phys. B **24**, 3091 (1991).
[6] N. Toshima, Phys. Lett. A **175**, 2024 (1993).
[7] D.R. Schultz, P.S. Krstic, C.O. Reinhold, and J.C. Wells, Phys. Rev. Lett. **76**, 2882 (1996).
[8] K.A. Hall, J.F. Reading, and A.L. Ford, J. Phys. B **29**, 6123 (1996).
[9] P.S. Krstic, D.R. Schultz, and R.K. Janev, J. Phys. B **29**, 1941 (1996).
[10] J.C. Wells, D.R. Schultz, P. Gavras, and M.S. Pindzola, Phys. Rev. A **54**, 593 (1996).
[11] ASACUSA Collaboration, CERN Report No. CERN/SPSC, 2002 (unpublished).
[12] A. Igarashi, S. Nakazaki, and A. Ohsaki, Phys. Rev. A **61**, 062712 (2000).
[13] B. Pons, Phys. Rev. Lett. **84**, 4569 (2000).
[14] B. Pons, Phys. Rev. A **63**, 012704 (2001).
[15] K. Sakimoto, J. Phys. B **33**, 3149 (2000).
[16] K. Sakimoto, J. Phys. B **33**, 5165 (2000).
[17] X.M. Tong, T. Watanabe, D. Kato, and S. Ohtani, Phys. Rev. A **64**, 022711 (2001).
[18] D.R. Schultz, J.C. Wells, P.S. Krstic, and C.O. Reinhold, Phys. Rev. A **56**, 3710 (1997).
[19] L.A. Wehrman, A.L. Ford, and J.F. Reading, J. Phys. B **29**, 5831 (1996).
[20] X.M. Tong and S.I. Chu, Chem. Phys. **217**, 119 (1997).
[21] X.M. Tong and S.I. Chu, Phys. Rev. A **61**, 021802 (2000).
[22] X.M. Tong and S.I. Chu, Phys. Rev. A **61**, 031401 (2000).
[23] X.M. Tong, D. Kato, T. Watanabe, and S. Ohtani, Phys. Rev. A **62**, 052701 (2000).
[24] X.M. Tong, D. Kato, T. Watanabe, and S. Ohtani, J. Phys. B **33**, 5585 (2000).
[25] G. Yao and S.I. Chu, Chem. Phys. Lett. **204**, 381 (1993).