Two- and one-center close-coupling calculations for ionization of atomic hydrogen by antiproton impact

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Ionization of atomic hydrogen by antiproton impact is studied by a two-center atomic-orbital close-coupling method supplementing projectile orbitals to the one-center expansion. Two-center effects are not negligible at intermediate and low energies, though antiprotons do not have bound states of electrons. The one-center expansion fails to represent the electron distribution near the antiproton where the electron tends to be evacuated by the repulsive interaction from the negatively charged nucleus. The integrated ionization cross sections are less sensitive to the details of the electron distribution, but below 1 keV the one-center expansion underestimates the ionization cross sections due to its inability to represent the expanding distribution of ionized electrons.

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An experimental facility called the Antiproton Decelerator (AD) has been built as an international cooperative project at CERN for the study of atomic collisions with slow antiprotons. In the near future, precise measurements of scattering cross sections of antiproton impact will be carried out and the unique physical character of the heavy negative ion will be investigated extensively. Theoretical studies of antiprotonic collisions are currently extremely popular.

One of the simplest nonperturbative approaches is the one-center atomic-orbital close-coupling (AOCC) calculation in the impact parameter formalism [1–3]. In this treatment, continuum states are replaced by the pseudocontinuum states obtained through the diagonalization of an atomic Hamiltonian. Since the antiproton has no bound states of electrons, this expansion has been generally believed to be accurate enough, in contrast with positive-ion impact cases, in which charge transfer plays a decisive role in the scattering. Toshima [4] extended the calculations utilizing the two-center atomic-orbital expansion method and compared them with those for proton impact. The continuum states belonging to the antiproton were incorporated in order to take explicit account of the effect in which the electron is repelled by the antiproton. In the above treatments, the pseudocontinuum states are square-integrable functions with finite ranges like the real bound states.

Pons [5] developed a new close-coupling scheme in which the scattering wave function is expanded as a linear combination of the spherical Bessel functions, which are the radial-part solutions of plane waves in the spherical coordinates. The basis functions are centered only on the hydrogen atom. The spherical Bessel functions have an infinite range, though they are confined in a box in order to discretize the continuum states in the practical calculations, and the restriction of the pseudocontinuum states is relaxed. It is not clear how well the two-center effect is taken into account in this method. He compared his results with those of the one-center pseudostate calculations and concluded that the total ionization cross sections do not differ much between the two types of calculations above the collision energy of 1 keV.

Wells *et al.* [6] solved time-dependent scattering equations directly on a three-dimensional Cartesian lattice. Though this method is free from the convergence problem of the basis functions, the approximate discretization on the lattice points brings about inaccuracy to the solutions. Besides, they had to confine the scattering system in a relatively small box in order to make the numerical calculations practically possible. They avoided the reflection of scattered waves at the boundaries by introducing an absorbing potential, the secondary effects of which are not yet understood well.

Sakimoto [7] treated only the radial motion of the heavy particles classically making the angular part coupled with that of the electron quantum mechanically. This method does not rely upon the traditional impact-parameter method so that the effect of the curved trajectory can be naturally introduced. The discrete-variable representation (DVR) was used for the numerical integration of the wave function.

Recently, Toshima [8] investigated the convergence problem of the pseudocontinuum states for the ionization of atomic hydrogen by proton impact employing huge numbers of pseudocontinuum states in three types of expansions, namely continuum states only on the target, only on the projectile, and on both of the nuclei. These three expansions show good agreement with one another at intermediate and low energies, indicating that the calculations are well converged. The addition of continuum states on the projectile accelerates the convergence considerably in comparison with the case in which continuum states are used only on the target. It is desirable to investigate the convergence problem also for the antiproton impact case.

In the present study, we extend the previous two-center calculations [4] enlarging the basis functions to check the convergence. (Atomic units are used throughout unless otherwise stated explicitly.) The number of states of the previous paper was not large enough to obtain good convergence and the incompleteness of the basis functions might have induced some undesirable instabilities to the cross sections [9]. The numerical procedure of the present close-coupling method is the same as the one used in previous studies [4,8]. The relative motion of the heavy particles is described classically by a rectilinear trajectory with a constant velocity v in

the impact-parameter representation. The time-dependent two-center electronic wave function is expanded in a standard way as

$$\Psi(\mathbf{r},t)=\sum_{i=1}^{N_T} a_i(t)\psi_i^T(\mathbf{r}_T,t)+\sum_{i=N_T+1}^{N} a_i(t)\psi_i^P(\mathbf{r}_P,t), \tag{1}$$

where $\psi_i^T(\mathbf{r}_T,t)$ and $\psi_i^P(\mathbf{r}_P,t)$ are the target and the projectile atomic orbital with appropriate electron translation factors attached, and $\mathbf{r}_T,\mathbf{r}_P$, and $\mathbf{r}$ are the electron coordinates measured from the target nucleus, from the projectile nucleus, and the coordinate origin, respectively. The eigenfunctions of each center are further expanded in terms of the Gaussian-type orbitals (GTO) as

$$\varphi_{nlm}(\mathbf{r})=\sum_{\nu} c_\nu^{n\ell} e^{-\alpha_\nu r^2} r^\ell Y_{\ell m}(\hat{r}), \tag{2}$$

where the nonlinear parameters α_ν are generated as a modified geometrical progression and the coefficients $c_\nu^{n\ell}$ are determined so as to diagonalize the atomic Hamiltonian of the target and the projectile. Since the interaction between the antiproton and the electron is repulsive, all the eigenenergies of the projectile are positive. It is not essential for the present study to know whether the basis functions are constructed from the Gaussian or from the Slater orbitals. Although the bound states of the hydrogen atom are also represented approximately as a linear combination of GTO, the energy eigenvalues are accurate enough to regard the states as exact.

At first, one-center calculations are carried out deleting the terms on the projectile (antiproton) in the expansion (1) to compare the present GTO expansion directly with the existing single-center calculations. The number of states and the range of the angular momentum are increased step by step to see the convergence. In the largest calculation, the basis set is composed of 656 states in the angular momentum range $0\leqslant\ell\leqslant12$. The ionization cross sections seem to converge quickly to reach a certain value for each collision energy. A smaller set with 354 states in the range $0\leqslant\ell\leqslant8$ gives almost identical ionization cross sections to those of the largest basis set, within a difference of a few percent. We coupled all the relavant magnetic quantum numbers fully without utilizing the dominance of small magnetic quantum numbers $0\leqslant m\leqslant3$ [3]. The apparently converged cross sections agree very closely at all the energies with the results of Igarashi [3], who used the Sturmian basis set for the expansion, but they differ somewhat from the other calculations [1,2]. Since the numbers of states employed in the present and Igarashi's calculations are much larger than the other two, we believe that our calculation produces better cross sections within the one-center expansion framework.

After seeing that the ionization cross sections do not change upon increasing further the number of states, continuum states are added stepwise for each ℓ on the antiproton. The ionization cross sections begin to change again slowly below 50 keV. Though the approximation of the straight-line trajectory might become unreliable below 1 keV [7], we extended the calculations down to 0.1 keV to see the two-center effect within the same approximation. At low energies, high angular momentum states are not needed on the projectile to achieve convergence, but their contribution increases as the collision energy becomes higher. 26 states with $0\leqslant\ell\leqslant2$ and 88 states with $0\leqslant\ell\leqslant4$ are used on the projectile below and above 1 keV, respectively. The difference between the one- and two-center calculations becomes prominent as the collision energy decreases below 1 keV. The results are shown in Fig. 1, in which other theoretical values and measurements are also given for comparison.

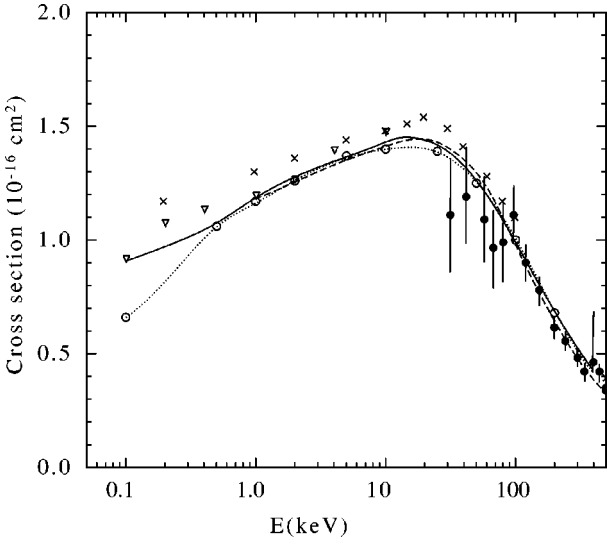

FIG. 1. Ionization cross sections of atomic hydrogen by antiproton impact. Solid line, present two-center GTO AOCC; dotted line, present one-center GTO AOCC; dashed line, spherical Bessel expansion [5]; circles, one-center Sturmian AOCC [3,10]; inverted triangles, DVR with straight-line trajectory [7]; crosses, lattice discretization [6]. Experimental data are from Knudsen *et al.* [11].

The disagreement with the two-center cross sections implies that the one-center calculations have not converged yet even for the largest basis set, though the difference is not so large above 1 keV. According to the variational principle, we can expect that the addition of new basis functions for the expansion always leads to an improvement of the wave function. Two factors can be considered as the cause of the difference between the two expansions.

At 0.1 keV, the two-center cross section is larger than the one-center one by a factor of 1.4. To see the convergence behavior, we show the ionization probabilities at 0.1 keV as a function of the impact parameter in Fig. 2. The addition of projectile *s* states changes the probabilities from the values of the apparently converged one-center expansion. The partial waves with $\ell=1$ and 2 on the projectile also contribute to the ionization. Higher partial waves $\ell\geqslant3$ have a negligible contribution. The integrated cross sections are 6.57×10^{-17}, 7.95×10^{-17}, 8.75×10^{-17}, and 8.94×10^{-17} cm^2 for the four probability curves, respectively, in order from bottom to top. At low energies, the average velocity of the ejected electron is larger than the incident velocity of the antiproton. The collision can be considered to have finished when the projectile and the target are separated by as much as 20 a.u. or so [5]. When the projectile energy is less than 1

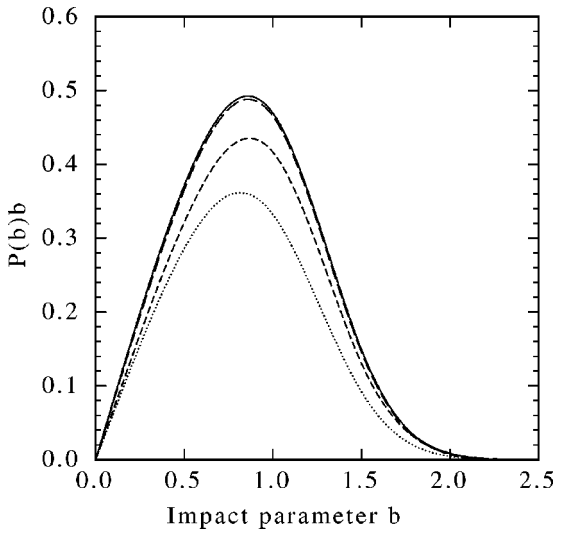

FIG. 2. Convergence behavior of the ionization probabilities of atomic hydrogen by antiproton impact at the collision energy 0.1 keV. Dotted line, one-center AOCC of 354 states. Other lines are two-center AOCC: 6 *s* states, 8 *p* states, and 12 *d* states are added step by step to the one-center basis set, shown by the short-dashed line, long-dashed line, and solid line, respectively.

keV, the electron spreads more than five times faster than the projectile on average and the electron cloud spreads as much as 100 a.u. or more. Such diffuse distribution cannot be expressed satisfactorily by the pseudocontinuum states of a standard size. However, the two-center expansion can take this situation into account to some extent by simulating the spreading electrons by the continuum states on the outgoing projectile. Igarashi [10] found that the ionization cross section increases gradually upon enlarging the size of the Sturmian basis functions below 1 keV. This finding supports the interpretation given above.

The difference at intermediate energies arises from a different mechanism. Due to the repulsive interaction, the electron tends to be evacuated near the antiproton. The necessity of the projectile states to take the repulsive interaction into account was pointed out in the previous paper [4]. Figure 3 shows the electron density distribution at the collision energy of 20 keV and the impact parameter $b=1.0$. The antiproton is located at the closest approach point, $(x,z)=(1.0,0.0)$. The electron density is integrated over the component perpendicular to the collision plane. The two-center calculations show dips in the distribution near the antiproton. In order to represent such a local structure of the wave function in the one-center expansion, we have to superimpose a large number of basis functions, both in the radial and the angular components. Even the largest basis set of the one-center expansion fails to produce the fine structure. The total ionization probability is less sensitive to the details of the wave function, thus we do not see a large discrepancy between the two expansions. The dip was also observed in the lattice calculations of Wells *et al.* [6]. In their results, the effect is much more prominent in a wider region. Though we cannot specify the reason for their enhanced dip, we point out that the confinement of the wave function in a small box affects

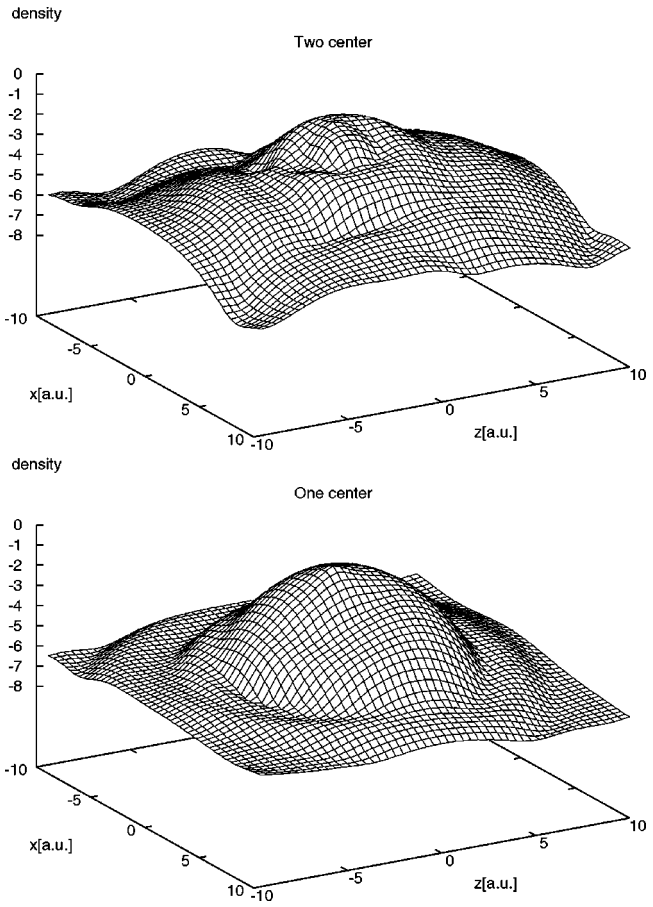

FIG. 3. Logarithmic plots of electron densities integrated over the component perpendicular to the collision plane. The incident beam is along the *z* axis and the impact parameter vector **b** is along the *x* axis. The two-center (top) and the one-center (bottom) expansions are compared at the collision energy 20 keV and the impact parameter $b=1.0$. The antiproton is located at the closest approach point, $(x,z)=(1.0,0.0)$.

the shape of the electron distribution. As the projectile velocity exceeds that of the electron, the collision time becomes short for the electron distribution to adjust its shape to the motion of the antiproton, hence the two-center effect tends to diminish.

New theoretical approaches have been developed for the study of ionization processes recently. Two of them [6,7] solve the Schrödinger equation directly without expanding the wave function, and the others [5,12] expand the wave function in terms of more flexible functions for the representation of continuum states. The former discretize the space coordinates to treat the continuous variables in a finite space. The discretization in the coordinate space is a counterpart of the basis expansion in the ordinary close-coupling method. The finite difference representation is based on a polynomial interpolation among the lattice points so that it can be regarded as an expansion of the scattering wave function in terms of local polynomials. The confinement in a finite box and the introduction of an absorbing potential induce secondary problems, as stated before. The latter two resolve the defect of pseudocontinuum states, which have a finite exten-

sion. These methods are superior to the traditional AOCC calculations for the study of the distribution of ionized electrons in coordinate space. Extension and refinement of these new approaches are desirable to complement research in the traditional close-coupling schemes.

To summarize, we investigated the convergence problem of AOCC by supplementing projectile states onto the one-center expansion. The electron distribution near the antiproton is not well represented by the one-center expansion, though this effect does not show up prominently in the total ionization cross sections. When the projectile velocity becomes much smaller than the electron velocity, the one-center expansion underestimates the ionization cross section due to its inability to represent the expanding electron distribution.

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