Time-dependent coupled-channel calculation for elastic scattering of positrons by hydrogen atoms and helium ions

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We investigate elastic scattering of positrons by hydrogen atoms and helium ions using a time-dependent coupled-channel (TDCC) method. Phase shifts are calculated with the time-energy Fourier transform of a wave packet. Numerical accuracy of the TDCC method is demonstrated for *S*-, *P*-, and *D*-wave scatterings by hydrogen atoms. For helium ions, we examine the low-lying *S*-wave resonances with a broad width recently predicted in variational eigenenergy calculations. However, resonancelike behaviors are not discernible in the *S*-wave phase shift for the ground-state target.

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I. INTRODUCTION

Recently, a time-dependent coupled-channel (TDCC) method [1] has been developed for Coulomb three-body systems, where a wave packet propagates in space and time. In this method, plenty of open and closed channels are automatically incorporated by numerically describing the radial wave functions without introducing overcomplete basis functions for the total wave function. Because of this advantage, the TDCC method has been successfully applied to many atomic processes: electron-impact excitation and ionization [2,3], autoionization [4], photoionization [5], dielectronic capture [6], rearrangement [7–9], and positron annihilation [10]. Integral cross sections are obtained for these inelastic processes by projecting the total wave packet onto bound states after the collision. However, this procedure is not adapted for calculations of differential cross sections, which needs phase shifts. Due to this reason, the TDCC method has not been applied to elastic scatterings, to our knowledge.

Positron scattering by hydrogenlike atoms, which is one of the simplest Coulomb three-body problems, provides a testing ground for theoretical methods used to study complex many-body problems. In the past decades, nonperturbed methods, the close-coupling [11], the *R*-matrix [12], the moment *T*-matrix [13], variational [14,15], and the convergent close-coupling [16] methods were developed to study positron scattering by hydrogen atoms, e.g., elastic scattering, excitation and ionization of atoms, and positronium (Ps) formation. However, some of those methods employ overcomplete expansion of total wave functions to incorporate a rearrangement channel, i.e., Ps channel. This treatment would cause pseudostructures, furthermore, pseudoresonances, in scattering cross sections. Therefore, the TDCC method is expected to be promising to treat positron scattering systems.

The positron-helium ion system is relatively simple, compared with the positron-hydrogen atom system, because of the different energy scales of the helium ion and Ps. In spite of this fact, in a variational calculation of eigenenergies with a stabilization method, Bhatia and Drachman [17] predicted that the system has two low-lying *S*-wave resonances with a broad width produced against the Coulomb repulsion between the positron and the helium ion. Their prediction was subsequently confirmed by Ho [18], and Ho and Yan [19] in a variational calculation of complex eigenenergies with a complex-coordinate rotation method; the position E_r and the width Γ were precisely determined to be $(E_r,\Gamma/2)=(-10.082,1.761)$ and $(-5.050,0.535)$ in eV. On the other hand, however, in a scattering calculation with a hyperspherical close-coupling method, Igarashi and Shimamura [20] raised an objection against existence of the broad resonances and instead reported narrow resonances supported by polarization force between the Ps and the helium nucleus. In a subsequent calculation with a close-coupling method, Bransden, Noble, and Whitehead [21] found no resonance. However, in a recent variational calculation with a coupled-rearrangement-channel method in which the complex-coordinate rotation method is incorporated, Toya [22] reproduced all resonances predicted partially by Bhatia and Drachman [17] and Igarashi and Shimamura [20]. The existence of the broad resonances are still controversial.

In the present paper, we study elastic scattering of positrons by hydrogen atoms and helium ions using the TDCC method. Numerical accuracy of the TDCC method is confirmed in calculations for hydrogen atoms; *S*-, *P*-, and *D*-wave phase shifts are calculated with the time-energy Fourier transform of a wave packet. For elastic scattering by helium ions, we calculate *S*-wave phase shift to search the broad resonances.

In the present paper, atomic units (a.u.) $e=m=\hbar=1$ are used unless otherwise stated.

II. TDCC METHOD FOR ELASTIC SCATTERING

The elastic-scattering cross section for the Jth partial wave is expressed with the *S*-matrix element as

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$$\sigma_{ii}^{J}(E)=\frac{\pi}{k^2}(2J+1)|1-S_{ii}(E)|^2, \tag{1}$$

where $S_{ii}(E)=e^{2i\delta_{ii}}$ with the elastic phase shift δ_{ii} and the total energy E. The S-matrix element is expressed as

$$\delta(E'-E)S_{fi}(E)=\langle\chi_f^-(E')|\chi_i^+(E)\rangle \tag{2}$$

in terms of the energy-normalized scattering wave functions $\chi_i^+(E)$ and $\chi_f^-(E')$ for incoming and outgoing asymptotic boundary conditions, where i and f denote the initial and final channels. The wave packet ψ_i and ψ_f are constructed from $\chi_i^+(E)$ and $\chi_f^-(E')$; for the incoming wave packet,

$$\psi_i=\int a_i(E)\chi_i^+(E)dE, \tag{3}$$

where $a_i(E)=\langle\chi_i^+(E)|\psi_i\rangle$ determines a scattering energy range. Since Eq. (3) can be inverted as $\chi_i^+(E)=a_i^{-1}(E)\delta(E-\hat{H})\psi_i$, we have an expression [23]

$$S_{fi}(E)=\frac{i}{2\pi a_i(E)a_f^*(E)}\langle\psi_f|G^+(E)|\psi_i\rangle,$$

$$=\frac{1}{2\pi a_i(E)a_f^*(E)}\int_0^\infty dt e^{iEt}C_{fi}(t), \tag{4}$$

where the energy-time Fourier transform for Green's function $G^+(E)$ and the correlation function $C_{fi}(t)=\langle\psi_f|e^{-i\hat{H}t}|\psi_i\rangle=\langle\psi_f|\psi(t)\rangle$ are used in the second line.

The three-body system of an electron, a positron, and a nucleus (a proton or a helium nucleus) are described by the Hamiltonian for relative motions given by

$$\hat{H}=\hat{T}+\hat{V}, \tag{5}$$

with the kinetic-energy operator

$$\hat{T}=\tfrac{1}{2}\hat{\boldsymbol{P}}^2+\tfrac{1}{2}\hat{\boldsymbol{p}}^2 \tag{6}$$

and the interaction operator

$$\hat{V}=\frac{-Z}{r}+\frac{Z}{R}+\frac{-1}{|\boldsymbol{R}-\boldsymbol{r}|}, \tag{7}$$

where Z is the nuclear charge, $\boldsymbol{R}$ and $\boldsymbol{r}$ the position vectors, respectively, of the positron and the electron from the nucleus, and $\hat{\boldsymbol{P}}$ and $\hat{\boldsymbol{p}}$ the conjugate momentum operators of $\boldsymbol{R}$ and $\boldsymbol{r}$, respectively. The total wave function with the total angular momentum J is expanded as

$$\Psi^{JM_J}(\boldsymbol{R},\boldsymbol{r},t)=\frac{1}{Rr}\sum_{Ll}\psi_{Ll}^{JM_J}(R,r,t)\mathcal{Y}_{Ll}^{JM_J}(\hat{\boldsymbol{R}},\hat{\boldsymbol{r}}) \tag{8}$$

over the angular-momentum eigenfunction

$$\mathcal{Y}_{Ll}^{JM_J}(\hat{\boldsymbol{R}},\hat{\boldsymbol{r}})=\sum_{Mm}C_{LM,lm}^{JM_J}Y_{LM}(\hat{\boldsymbol{R}})Y_{lm}(\hat{\boldsymbol{r}}), \tag{9}$$

where L and l are the angular momenta associated with $\hat{\boldsymbol{R}}$ and $\hat{\boldsymbol{r}}$, respectively, Y_{lm} the spherical harmonics, and $C_{LM,lm}^{JM_J}$ the Clebsch-Gordan coefficient. The TDCC equation for the radial part of the wave function is derived to be

$$i\frac{\partial}{\partial t}\psi_{Ll}^{JM_J}(R,r,t)=\sum_{L'l'}[\hat{T}_{Ll}^{JM_J}\delta_{LL'}\delta_{ll'}+\hat{V}_{LlL'l'}^{JM_J}]\psi_{L'l'}^{JM_J}(R,r,t), \tag{10}$$

where

$$\hat{T}_{Ll}^{JM_J}=-\frac{1}{2}\frac{\partial^2}{\partial R^2}+\frac{L(L+1)}{2R^2}-\frac{1}{2}\frac{\partial^2}{\partial r^2}+\frac{l(l+1)}{2r^2} \tag{11}$$

and

$$\hat{V}_{LlL'l'}^{JM_J}=\langle\mathcal{Y}_{Ll}^{JM_J}|\hat{V}|\mathcal{Y}_{L'l'}^{JM_J}\rangle$$

$$=\frac{-Z}{r}+\frac{Z}{R}-(-1)^{L'+l+J}\hat{L}\hat{l}$$

$$\times\sum_k\frac{r_<^k}{r_>^{k+1}}\begin{Bmatrix}L & l & J\\ l' & L' & k\end{Bmatrix}C_{L0k0}^{L'0}C_{l0L0}^{l'0}. \tag{12}$$

We introduce a variable transform technique [9,24] to accurately describe wave functions. The radial coordinates R and r are nonlinearly scaled by variables X and x,

$$R=F(X),\qquad r=f(x), \tag{13}$$

with appropriate functions F and f. Accordingly, the radial wave function is transformed into

$$\tilde{\psi}_{Ll}^{JM_J}(X,x,t)=\sqrt{F'f'}\,\psi_{Ll}^{JM_J}(R,r,t) \tag{14}$$

and, at the same time, the differential operators of Eq. (11) as

$$\frac{\partial^2}{\partial R^2}\to\frac{1}{F'}\frac{\partial^2}{\partial X^2}\frac{1}{F'}+\frac{1}{2}\frac{F'''}{F'^3}-\frac{3}{4}\frac{F''^2}{F'^4}, \tag{15}$$

$$\frac{\partial^2}{\partial r^2}\to\frac{1}{f'}\frac{\partial^2}{\partial x^2}\frac{1}{f'}+\frac{1}{2}\frac{f'''}{f'^3}-\frac{3}{4}\frac{f''^2}{f'^4}. \tag{16}$$

III. NUMERICAL METHOD

The radial wave function is numerically described over $N^2=600^2$ or 800^2 grid points in the two-dimensional (X,x) plane. The grid points are uniformly taken up to $X_{\max}=x_{\max}=16\lambda$ or 20λ with spacings of $\Delta X=\Delta x=X_{\max}/N$, where λ denotes de Broglie wavelength of an incident positron. The scaling functions are given by

$$F(X)=X[1-A\exp(-BX)], \tag{17}$$

$$f(x)=x[1-a\exp(-bx)], \tag{18}$$

where the parameters are taken as

$$A=(1-\Delta R/\Delta X)\exp(B\Delta X),\quad B=2/X_{\max},$$

TABLE I. Convergence of *S*-, *P*-, and *D*-wave cross sections for positron-hydrogen elastic scattering with respect to $l_{\max}$ in the wave-function expansion (8).

	E_{e^+} (eV)	$l_{\max}$ 5	7	9
	1	1.260	1.408	1.585
	5	0.001	0.000	0.000
S wave	10	0.098	0.091	0.087
	30	0.152	0.151	0.151
	50	0.133	0.132	0.131
	1	0.386	0.439	0.457
	5	0.657	0.718	0.745
P wave	10	0.450	0.476	0.490
	30	0.060	0.062	0.063
	50	0.052	0.052	0.052
	1	0.012	0.013	0.013
	5	0.131	0.162	0.168
D wave	10	0.413	0.416	0.425
	30	0.103	0.106	0.107
	50	0.045	0.045	0.046

$$a=(1-\Delta r/\Delta x)\exp(b\Delta x), \quad b=2/x_{\max},$$

and

$$\Delta R=\Delta r=0.1/Z.$$

The grid points in the (R,r) plane are dense in a collision region while sparse in an asymptotic region. With these scaling functions, an accuracy better than 0.1% is obtained for the energy eigenvalue of the ground-state hydrogen atom [9].

The initial condition for the TDCC equation (10) is set as

$$\psi_{Ll}^{JM_J}(R,r,t_0)=g_{kL}(R)\phi_{1s}(r)\delta_{LJ}\delta_{l0}, \tag{19}$$

with the ground-state wave function $\phi_{1s}(r)$ of the target hydrogen atom or helium ion and an incoming wave packet of the positron,

$$g_{kL}(R)=\frac{1}{(w^2\pi)^{1/4}}\exp\left[-\frac{(R-R_0)^2}{2w^2}\right]\phi_{kL}(R), \tag{20}$$

where k is a wave number of the incident positron and w is a width of the wave packet. The incoming wave function $\phi_{kL}(R)$ is taken to be an asymptotic form of the spherical Hankel function for a neutral target or of the Coulomb function [25] for a charged target. The parameters are taken as $R_0=F[X=(3/4)X_{\max}]$ and $w=1.5\lambda$. The time evolution is traced for a time $t_{\max}\gg 2R_0/k$. An absorption potential [26] is put at the boundary $X=X_{\max}$ to not induce artificial reflection of the wave. The TDCC equation (10) is fast and stably solved with the split-operator method developed in Ref. [8]. The expansion in Eq. (8) is truncated by the upper limit $l_{\max}$ of the electron angular momentum l; for a given l, the positron angular momentum L takes all possible values that satisfy the conservation of angular momentum $|J-l|\leqslant L\leqslant J+l$ and parity $\Pi=(-1)^{L+l}=(-1)^J$.

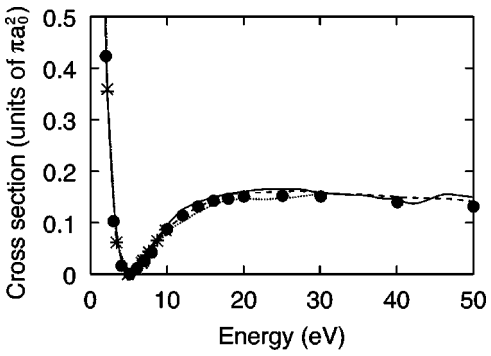

FIG. 1. *S*-wave cross section for positron-hydrogen elastic scattering. Closed circles represent the present result; solid line, the 18-state close-coupling method [11]; broken line, the intermediate energy *R*-matrix method [12]; dotted line, the moment *T*-matrix method [13]; crosses, a variational method with Hylleraas basis functions [14]; and pluses, the Harris-Nesbet variational method [15].

The *S*-matrix element of elastic scattering is obtained by taking ψ_f to be a delta function $\delta(R-R_\infty)$ times an outgoing asymptotic radial function $\phi_{kL}(R)\phi_{1s}(r)$ as

$$S_{ii}(E)=\frac{i}{a_i(E)}\sqrt{\frac{k}{2\pi}}\phi_{kL}^*(R_\infty)\int_0^\infty dt e^{iEt}\langle\phi_{1s}|\psi(t)\rangle_{R=R_\infty}, \tag{21}$$

where R_∞ is a fixed radial coordinate in the asymptotic region. Equation (21) is very useful, because the matrix element can be calculated for several scattering energies provided by $a_i(E)$ from one wave-packet propagation.

IV. RESULTS AND DISCUSSION

A. Positron scattering by hydrogen atoms

We check convergences of *S*-, *P*-, and *D*-wave elastic cross sections for hydrogen atom targets with respect to $l_{\max}$ in the wave-function expansion (8). Table I shows that cross sections sufficiently converge for high energy, but convergence becomes slow for low energy; the change of values of

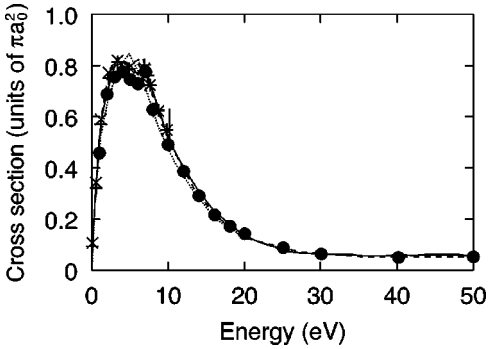

FIG. 2. *P*-wave cross section for positron-hydrogen elastic scattering. The notation is the same as in Fig. 1.

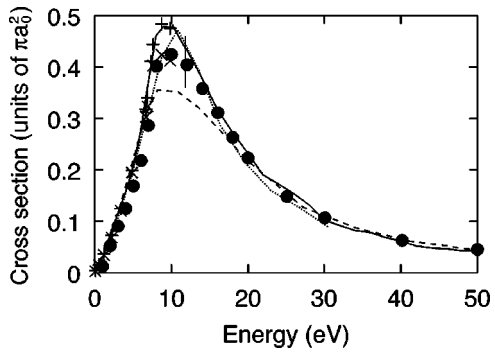

FIG. 3. *D*-wave cross section for positron-hydrogen elastic scattering. The notation is the same as in Fig. 1.

cross sections from $l_{max}=7-9$ is 11% at 1 eV for the *S* wave and 4% below 5 eV for the *P* and *D* waves. The uncertainty coming from number and spacing of grid points is sufficiently small. Therefore, the numerical accuracy of the calculation is estimated to be better than several percents except for 1 eV for the *S* wave.

Figures 1–3 show *S*-, *P*-, and *D*-wave elastic cross sections, respectively. For the *S* wave, the present result is in excellent agreement with previous results obtained with the close-coupling [11], the *R*-matrix [12], the moment *T*-matrix [13], a variational [14], and the Harris-Nesbet variational [15] methods. The Ramsauer-Townsend minimum at 5 eV is accurately reproduced in the present calculation. For the *P* wave, the present result is in good agreement with the previous results above 10 eV, but slightly deviates, about 5% smaller, around 5 eV where the cross section has a maximum. This underestimation is considered to come from the slow convergence of the cross section with respect to l_{max}. The present calculation reproduces a cusp structure at the Ps formation threshold (6.8 eV) confirmed in some of the previous calculations. For the *D* wave, the present result is in good agreement with previous results at energies higher than 15 eV. Around 10 eV, where the cross section has a maximum, the present result agrees well with the result of a variational calculation [14], but deviates from other results: about

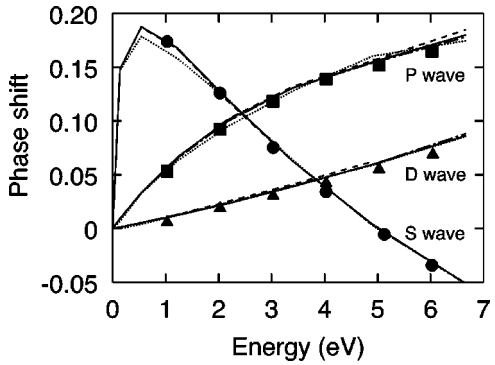

FIG. 4. *S*-, *P*-, and *D*-wave phase shifts for positron-hydrogen elastic scattering. Closed symbols represent the present result; solid line, a variational method with Hylleraas basis functions [14]; broken line, the intermediate energy R-matrix method [12]; dotted line, the moment *T*-matrix method [13]; and dash-dotted line, the Harris-Nesbet variational method [15].

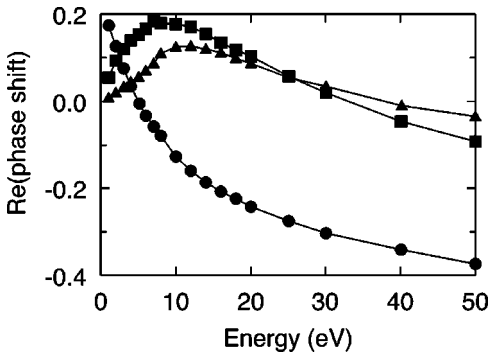

FIG. 5. Real part of phase shifts for positron-hydrogen elastic scattering. Closed circles, squares, and triangles represent *S*-, *P*-, and *D*-wave phase shifts, respectively.

15% larger than the intermediate energy *R*-matrix calculation [12] and 15% smaller than the close-coupling [11], the moment *T*-matrix [13], and the Harris-Nesbet [15] calculations.

Figure 4 shows the comparison of elastic phase shifts with the previous results [12–15] below the Ps-formation threshold. For the *S* wave, the present result is in excellent agreement with the previous results similar to the agreement in cross sections (see Fig. 1). However, for the *P* and *D* waves, the present results somewhat deviate, about 3% lower, from the previous results. This small deviation may indicate that in the present calculation attractive polarization force is not sufficiently incorporated, i.e., the completeness of the wave-function expansion is not sufficient in comparison with previous calculations. Thus, the deviation is expected to be improved by taking a larger value of l_{max}.

Figures 5 and 6 show the real and imaginary parts of elastic phase shifts. The real part of the *S*-wave phase shift monotonically decreases as the energy increases and becomes negative at energies higher than 5 eV. The negative phase shift indicates that the interaction between the positron and the hydrogen atom is dominated by the static Coulomb repulsion. The imaginary part monotonically increases as the energy increases from the Ps-formation threshold. For *P* and *D* waves, the real parts of the phase shifts have a maximum around 10 eV and become positive at energies lower than about 35 eV. In this energy region, the interaction between the positron and the hydrogen atom is dominated by an attractive force coming from target polarization.

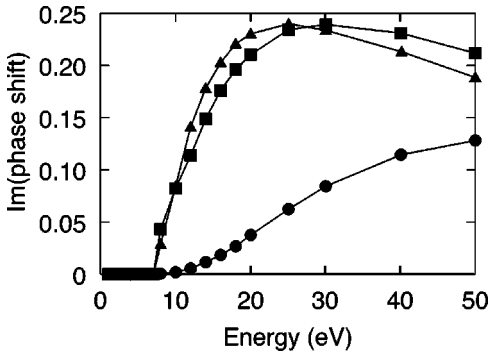

FIG. 6. Imaginary part of phase shifts for positron-hydrogen elastic scattering. The notation is the same as in Fig. 5.

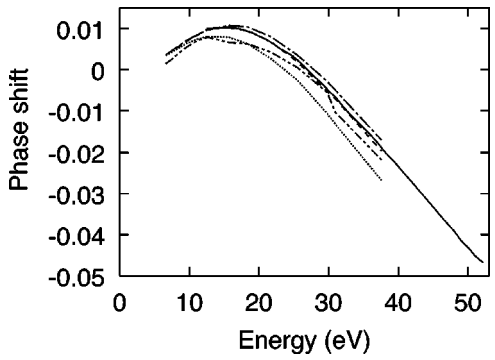

FIG. 7. *S*-wave phase shift for positron-helium ion elastic scattering. The solid line represents the present result; broken line, the 29-state close-coupling method [21]; dash-dotted line, the Harris-Nesbet variational method [27]; dash-double dotted line, the Harris method [28]; and dotted line, the polarized orbital approximation [29].

B. Positron scattering by helium ions

Figure 7 shows *S*-wave elastic phase shifts for helium ion targets; the present result has been given at positron energies of every 1 eV from 13 eV to 52 eV. Although the phase shift is one order of magnitude smaller than that for hydrogen atom targets, the present result is in excellent agreement with previous results obtained with the 29-state close-coupling method [21] and the Harris-Nesbet variational method [27]. This agreement indicates high numerical accuracy of the TDCC method. However, the Harris method [28] gives good agreement at energies higher than 25 eV, but lower values of phase shifts at energies lower than 25 eV. The polarized-orbital approximation [29] gives lower values at energies higher than 10 eV. The result of the hyperspherical close-coupling method by Igarashi and Shimamura [20] significantly deviates from the present result; in the cross section, their results at 47.62 eV and 52.57 eV are about factor of 2.5 larger than the present result. This overestimation has been also pointed out by Bransden, Noble, and Whitehead [21].

The *S*-wave phase shift monotonically decreases as the energy increases around the energy position of the two broad resonances, 44.34 eV and 49.37 eV, predicted by Bhatia and Drachman [17] and confirmed by Ho [18], Ho and Yan [19], and Toya [22]; the positions are relative to the ground-state energy of helium ions. The phase shift should rise suddenly around the energy position of the resonances. However, no rise of the phase shift is seen in Fig. 7. Moreover, the interaction between the positron and the helium ion turns out to be repulsive in view of negative values of the phase shift. Therefore, the broad resonances are not discernible in elastic scattering of positrons by ground-state helium ions.

V. SUMMARY

We have applied the TDCC method to elastic scattering of positrons by ground-state hydrogen atoms and helium ions. In the scattering by hydrogen atom, the present result for the partial cross section and the phase shift exhibits excellent agreement with previous results for the *S* wave, and good agreement for the *P* and *D* waves. In the scattering by helium ion, we have searched the *S*-wave phase shift for broad resonances predicted, but found no behavior suggesting them.

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[1] C. Bottcher, J. Phys. B **14**, L349 (1981); Adv. At. Mol. Phys. **20**, 241 (1985).

[2] M.C. Witthoeft, M.S. Pindzola, and J. Colgan, Phys. Rev. A **67**, 032713 (2003); M.S. Pindzola and F.J. Robicheaux, *ibid.* **61**, 052707 (2000); M.S. Pindzola and F. Robicheaux, *ibid.* **54**, 2142 (1996); W. Ihra, M. Draeger, G. Handke, and H. Friedrich, *ibid.* **52**, 3752 (1995).

[3] V.V. Serov, B.B. Joulakian, D.V. Pavlov, I.V. Puzynin, and S.I. Vinitsky, Phys. Rev. A **65**, 062708 (2002); V.V. Serov, V.L. Derbov, B.B. Joulakian, and S.I. Vinitsky, *ibid.* **63**, 062711 (2001).

[4] D.R. Schultz, C. Bottcher, D.H. Madison, J.L. Peacher, G. Buffington, M.S. Pindzola, T.W. Gorczyca, P. Gavras, and D.C. Griffin, Phys. Rev. A **50**, 1348 (1994).

[5] J. Colgan and M.S. Pindzola, Phys. Rev. A **67**, 012711 (2003); **65**, 032729 (2002); M.S. Pindzola and F. Robicheaux, *ibid.* **57**, 318 (1998).

[6] D.M. Mitnik, D.C. Griffin, and M.S. Pindzola, Phys. Rev. Lett. **88**, 173004 (2002).

[7] D.R. Plante and M.S. Pindzola, Phys. Rev. A **57**, 1038 (1998).

[8] N. Yamanaka and Y. Kino, Phys. Rev. A **64**, 042715 (2001); Hyperfine Interact. **138**, 85 (2001); Nucl. Instrum. Methods Phys. Res. B (to be published).

[9] N. Yamanaka and Y. Kino, Phys. Rev. A **65**, 062709 (2002).

[10] N. Yamanaka, Y. Kino, Y. Takano, H. Kudo, and A. Ichimura, Phys. Rev. A **67**, 052712 (2003); N. Yamanaka and Y. Kino, in Proceedings of the third European Conference on Atomic Physics at Accelerators (APAC2001), Aarhus, Denmark [Hyperfine Interact. (to be published)]; http://nucl.phys.s.u-tokyo.ac.jp/yam/tdcc/

[11] A.A. Kernoghan, D.J.R. Robinson, M.T. McAlinden, and H.R.J. Walters, J. Phys. B **29**, 2089 (1996); A.A. Kernoghan, M.T. McAlinden, and H.R.J. Walters, *ibid.* **28**, 1079 (1995).

[12] K. Higgins and P.G. Burke, J. Phys. B **26**, 4269 (1993); **24**, L343 (1991); K. Higgins, P.G. Burke, and H.R.J. Walters, *ibid.* **23**, 1345 (1990).

[13] J.R. Winick and W.P. Reinhardt, Phys. Rev. A **18**, 910 (1978); **18**, 925 (1978).

[14] J.W. Humberston, Can. J. Phys. **60**, 591 (1982); J. Phys. B **17**, 2353 (1984); C.J. Brown and J.W. Humberston, *ibid.*, **17**, L423

(1984); **18**, L401 (1985); D. Register and R.T. Poe, Phys. Lett. **51A**, 431 (1975); A.K. Bhatia, A. Temkin, and H. Eiserike, Phys. Rev. A **9**, 219 (1974); A.K. Bhatia, A. Temkin, R.J. Drachman, and H. Eiserike, *ibid.* **3**, 1328 (1971).

[15] Y.R. Kuang and T.T. Gien, Phys. Rev. A **55**, 256 (1997); T.T. Gien, *ibid.* **56**, 1332 (1997); **59**, 1238 (1999).

[16] A.S. Kadyrov and I. Bray, Phys. Rev. A **66**, 012710 (2002).

[17] A.K. Bhatia and R.J. Drachman, Phys. Rev. A **42**, 5117 (1990).

[18] Y.K. Ho, Phys. Rev. A **53**, 3165 (1996).

[19] Y.K. Ho and Z.-C. Yan, Phys. Rev. A **66**, 062705 (2002).

[20] A. Igarashi and I. Shimamura, Phys. Rev. A **56**, 4733 (1997).

[21] B.H. Bransden, C.J. Noble, and R.J. Whitehead, J. Phys. B **34**, 2267 (2001).

[22] Y. Toya, Ph.D. thesis, Tohoku University, 2003 (unpublished).

[23] J. Zeng and H. Zhang, *Theory and Application of Quantum Molecular Dynamics* (World Scientific, Singapore, 1999), Chap. 7.

[24] I. Kawata and H. Kono, J. Chem. Phys. **111**, 9498 (1999); I. Kawata, H. Kono, and Y. Fujimura, *ibid.* **110**, 11 152 (1999).

[25] *Computational Atomic Physics: Electron and Positron Collisions with Atoms and Ions*, edited by K. Bartschat (Springer, Berlin, 1996), Chap. 9.

[26] S. Brouard, D. Macías, and J.G. Muga, J. Phys. A **27**, L439 (1994); D. Macías, and S. Brouard, and J.G. Muga, Chem. Phys. Lett. **228**, 672 (1994); J.P. Palao, J.G. Muga, and R. Sala, Phys. Rev. Lett. **80**, 5469 (1998); J.P. Palao and J.G. Muga, J. Phys. Chem. A **102**, 9464 (1998).

[27] T.T. Gien, J. Phys. B **34**, L535 (2001).

[28] I. Shimamura, J. Phys. Soc. Jpn. **31**, 217 (1971).

[29] P. Khan, Z. Phys. A **318**, 19 (1984).