Momentum-space coupled-channel optical method for positron-hydrogen scattering

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The scattering of positrons from atomic hydrogen is studied by using the momentum space coupled channels optical method at intermediate energy (15–100 eV). Ionization continuum and positronium formation channels are included in the coupled channels calculation via a complex equivalent-local optical potential.

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I. INTRODUCTION

In recent years, theoretical studies on positron-hydrogen collision systems have reached a level where positronium formation channels can be taken into account for comparison with experimental measurements. These calculations were mainly performed in the close coupling framework at lower and some intermediate energies (Hewitt *et al.* [1], Mitroy [2], and Kernoghan *et al.* [3]). The scattering cross sections obtained by these calculations are in good agreement with the corresponding experimental measurements (Zhou *et al.* [4]). In the highly interesting intermediate energy regime, the ionization continuum forms a significant part that contributes to the total scattering cross section. Considerable advances in theoretical studies of positron-atom collision have been made by Mitroy [2] and Kernoghan *et al.* [3] by employing a L^2 representation to describe the excitation of the target continuum in their close coupling calculations. Most recently, Kadyrov and Bray [5] reported a convergent two-center close-coupling approach, they found that the major cross sections do convergent if sufficient number of pseudostates are used to expand the total scattering wave function. These results of pseudostate expansion calculation have shown that the scattering cross sections depend on the size and l values of the L^2 bases.

The momentum space coupled channels optical method (CCO) for electron-atom scattering was developed in the 1980s (McCarthy and Stelbovics [6,7]) using an extreme screening approximation to describe the three-body breakup process. It has given excellent ionization cross sections for positron scattering by hydrogen (Ratnavelu [8]). The CCO method for electron scattering solves the coupled integral equations for discrete channels (P space) to convergence using a coupling potential that includes an *ab initio* polarization part describing the real and virtual excitation of the continuum of Q space. With different levels of detail the method has had broad success for atoms whose structure can be described by one or two active electrons, but extending the method to the studies of positron-atom scattering requires developments in the method.

In the positron-atom system two physically distinct mechanisms contribute to the positron-atom interaction. The first one is the dynamic polarization of the target by the positron. The interaction is roughly proportional to the atomic dipole polarizability α at large distances. The second mechanism is the formation of positronium bound states by the positron and one of the valence electrons. The total positron-atom polarization potential is the sum of the target-polarization potential and the positronium formation potential. The description of positron scattering by atom must include a complex polarization potential: the real part describes virtual excitation of the target continuum and the virtual formation of positronium, the imaginary part describes real excitation of these channels and the formation of positronium bound states.

In the present work, we report studies of positron-hydrogen scattering at energy ranging from 15 to 100 eV, using the momentum space coupled channels method, in which we solve coupled integral equations for discrete channels in P space. We have developed an equivalent-local complex potential describing the rearrangement process, namely positronium (Ps) formation, that is added to an *ab initio* polarization part, extending the momentum space coupled channels optical method to positron-atom systems. A check for the validity of the method for a particular target is its ability to generate accurate cross sections for all channels: total ionization cross section, positronium formation cross section, total cross section and differential and integrated cross sections for P-space physical channels.

II. THEORETICAL METHOD

The *Schrödinger* equation for positron scattering on an atom target is

$$[E - (K_p + H_T + V)]|\Psi_n^{\pm}\rangle = 0, \tag{1}$$

where E is the total scattering energy, K_p stands for the kinetic energy of the positron, H_T is the target Hamiltonian, and V is the positron-target potential operator,

$$V = V_0 + V_{pe}, \tag{2}$$

here V_{pe} is the interaction between the incident positron and the active electron of the target and V_0 is the interaction of the positron with an inert core consisting of the nucleus and the remaining electrons. $\Psi_n^{\pm}$ is the total scattering wave function for the channel n. The superscripts ± denote outgoing and ingoing spherical wave boundary conditions, respectively. $\Psi_n^{\pm}$ consists of two parts representing the excitation of

target states $\psi_l(\mathbf{r}_e)$ and positronium states $\Phi_\mu(\mathbf{k}_{Ps},\mathbf{R},\mathbf{r})$,

$$\Psi_n^{\pm} = \sum_l \psi_l(\mathbf{r}_e)F_l(\mathbf{r}_p) + \sum_\mu \Phi_\mu(\mathbf{k}_{Ps},\mathbf{R},\mathbf{r}), \tag{3}$$

where $\mathbf{r}_p,\mathbf{r}_e$ are the coordinates of the positron and the electron. The relative coordinate is

$$\mathbf{r} = \mathbf{r}_p - \mathbf{r}_e, \tag{4}$$

and $\mathbf{R}$ is the coordinate of the positronium center of mass and

$$\mathbf{R} = \frac{1}{2}(\mathbf{r}_p + \mathbf{r}_e). \tag{5}$$

$\mathbf{k}_{Ps}$ is the momentum of center of mass of the positronium formation. We use projection operators P and Q for the sets of channel states ψ_i

$$P = \sum_{i\in P} |\psi_i\rangle\langle\psi_i|, \tag{6}$$

$$Q = 1 - P. \tag{7}$$

The coupled channels optical equation (McCarthy and Stelbovics [7]) is

$$\langle \mathbf{k}i|T|0\mathbf{k}_0\rangle = \langle \mathbf{k}i|V^{(Q)}|0\mathbf{k}_0\rangle + \sum_{j\in P}\int d^3k'\langle \mathbf{k}i|V^{(Q)}|j\mathbf{k}'\rangle \times \frac{1}{E^{(+)} - \varepsilon_j - \frac{1}{2}k'^2}\langle \mathbf{k}'j|T|0\mathbf{k}_0\rangle, \quad i\in P. \tag{8}$$

The channel states in P space are a finite set including the entrance channel $|0\rangle$. The target states are defined by the target Hamiltonian H_T,

$$(\varepsilon_j - H_T)|\psi_j\rangle = 0. \tag{9}$$

The target ionization continuum and the discrete positronium-formation channels are represented in Q space via an optical potential, which is the channel coupling potential V plus the polarization potential $W^{(Q)}$,

$$V^{(Q)} = V + W^{(Q)}, \tag{10}$$

$$W^{(Q)} = W_I^{(Q)} + W_{Ps}^{(Q)}. \tag{11}$$

Here $W_I^{(Q)}$ and $W_{Ps}^{(Q)}$ stand for the parts of the polarization potential that describe the ionization continuum and positronium formation rearrangement process, respectively. The form used for the matrix element of the polarization potential $W_I^{(Q)}$ describing ionization is (McCarthy and Zhou [9])

$$\langle \mathbf{k}'i|W_I^{(Q)}|j\mathbf{k}\rangle = \sum_{n\in Q}\langle \mathbf{k}'i|V|\chi_n^{(-)}\rangle\frac{1}{E^{(+)} - E_n}\langle\chi_n^{(-)}|V|j\mathbf{k}\rangle, \tag{12}$$

where $|\chi_n^{(-)}\rangle$ represents the distorted wave function for the reaction starting in channel n. The notation n is a discrete notation for the three-body ionization continuum. For ionization states we use the extreme screening approximation

$$|\chi_n^{(-)}\rangle = |\varphi^{(-)}(\mathbf{q}_<)\mathbf{q}_>\rangle, \tag{13}$$

where $\mathbf{q}_<$ and $\mathbf{q}_>$ are the momenta of the outgoing particles with greater and lesser absolute values, respectively. Ionization is described in the independent particle model, $\langle\mathbf{r}|\varphi^{(-)}(\mathbf{q}_<)\rangle$ is a Coulomb wave orthogonalized to orbital from which the electron is removed. $\langle\mathbf{r}|\mathbf{q}_>\rangle$ is a plane wave.

The model used for Ps formation is

$$|\chi_n^{(-)}\rangle = \phi_\mu e^{i\mathbf{k}_{Ps}\cdot\mathbf{R}}, \tag{14}$$

where ϕ_μ is the bound state of the positronium, and $\mathbf{k}_{Ps}$ is the momentum of the positronium center of mass. The plane wave $\langle\mathbf{R}|\mathbf{k}_{Ps}\rangle$ represents the motion of positronium, since only short-range terms in the positronium-ion potential survive. The notation n is a discrete notation for the two-body Ps rearrangement channels.

The optical potential for positronium formation is

$$\langle \mathbf{k}'i|W_{Ps}^{(Q)}|j\mathbf{k}\rangle = \sum_\mu \langle \mathbf{k}'i|V|\tilde{\chi}_n^{(-)}\rangle\frac{1}{E^{(+)} - \varepsilon_n - k_{Ps}^2}\langle\tilde{\chi}_n^{(-)}|V|j\mathbf{k}\rangle. \tag{15}$$

Here

$$|\tilde{\chi}_n^{(-)}\rangle = (1 - |\psi_i\rangle\langle\psi_i|)|\chi_n^{(-)}\rangle, \tag{16}$$

$|\chi_n^{(-)}\rangle$ is orthogonalized to the ground state of hydrogen atom, and $|\psi_i\rangle$ from which the electron is captured.

The amplitudes of positronium formation potential coincides with the one obtained using atomic many-body theory (Gribakin and King [10]). It has been calculated by using the numerical method of Cheshire [11].

A half-on-shell equivalent-local approximation is made for the positronium formation potential and the optical potential matrix element is calculated only at about ten points in the variable K, where

$$K = |\mathbf{k} - \mathbf{k}'|, \quad \frac{1}{2}k^2 = E - \varepsilon_0, \quad \frac{1}{4}k_{Ps}^2 + \varepsilon_{Ps} = \frac{1}{2}k^2 + \varepsilon_0. \tag{17}$$

This is achieved by an angular-momentum projection

$$\langle \mathbf{k}'i|W^{(Q)}|j\mathbf{k}\rangle = \sum_{l''m''} C_{l'l''l}^{m'm''m}U_{l'l''l}(K)Y_{l''m''}(\hat{\mathbf{K}}),$$

$$U_{l'l''l}(K) = \sum_{m'm''} C_{l'l''l}^{m'm''m}\int d\hat{\mathbf{k}}\langle \mathbf{k}'i|W^{(Q)}|j\mathbf{k}\rangle i^{-l''}Y_{l''m''}^*(\hat{\mathbf{K}}).$$

Cubic spline interpolation is used for general values of K.

The equivalent-local complex potential is calculated by a multidimensional method using Cartesian momentum variables (McCarthy and Stelbovics [6]). The real part for ionization involves virtual (off-energy-shell) excitation into Q space, the real part for positronium formation describes virtually-formed positronium bound states with the positron bound to the valence electron.

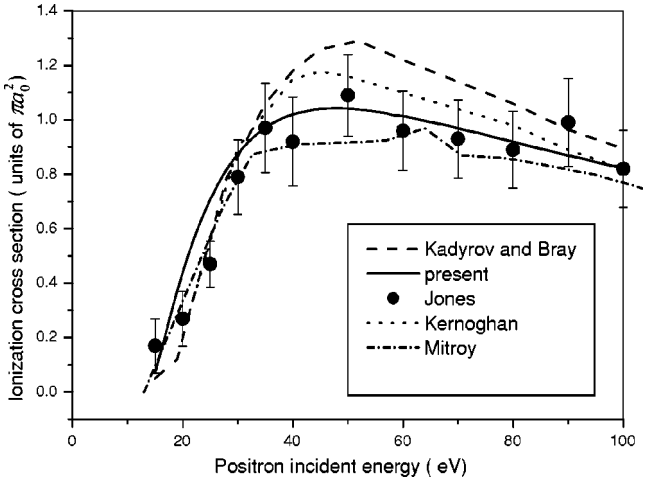

FIG. 1. Ionization cross section for positron impact on hydrogen (πa_0^2). The solid line: present calculation; the short dash dot line: L^2 calculation (Mitroy [2]); the long dash line: two-center convergent close-coupling result of Kadyrov and Bray [5]; the dot line: calculation of Kernoghan *et al.* [3]; the experimental data: Jones *et al.* [12].

A simple estimate of the total cross section for exciting Q space is

$$\sigma_Q = \left(\frac{2}{k}\right)(2\pi)^3 \,\mathrm{Im}\langle \mathbf{k}0|W^{(Q)}|0\mathbf{k}\rangle, \tag{18}$$

where $|0\rangle$ stands for the ground state of the target. The total ionization cross section is

$$\sigma_I = \left(\frac{2}{k}\right)(2\pi)^3 \,\mathrm{Im}\langle \mathbf{k}0|W_I^{(Q)}|0\mathbf{k}\rangle. \tag{19}$$

The total positronium formation cross section is

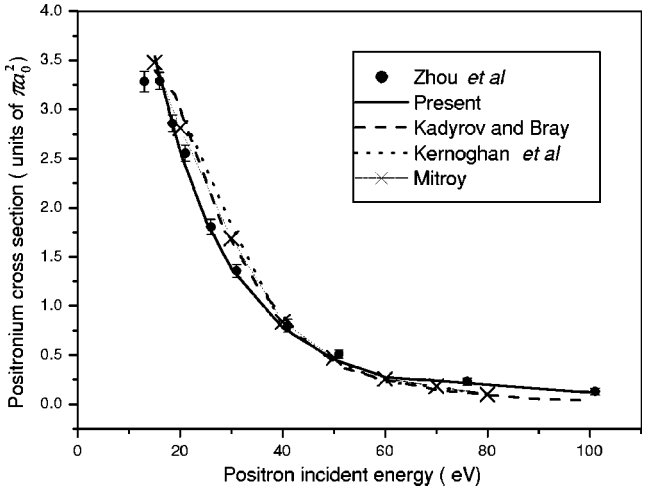

FIG. 2. Positronium formation cross section for positron scattering by hydrogen (πa_0^2). The solid line: present calculation; the line with symbol $\times$: L^2 calculation of Mitroy [2]; the long dash line: two-center convergent close-coupling result of Kadyrov and Bray [5]; the dot line: calculation from Kernoghan *et al.* [3]; experimental data from Zhou *et al.* [4].

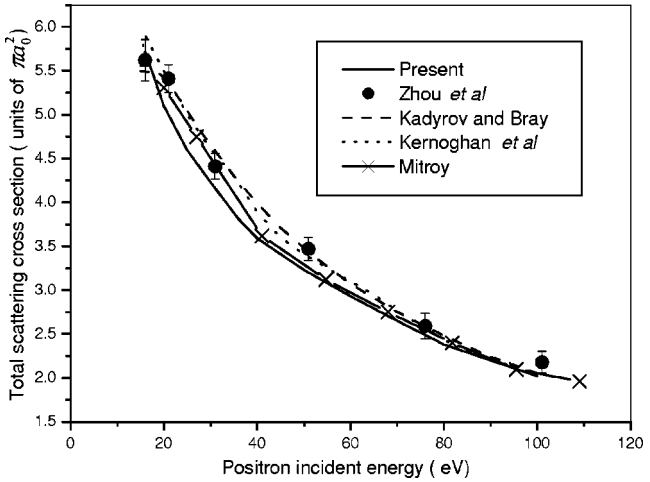

FIG. 3. Total cross section for positron scattering by hydrogen (πa_0^2). The notations are the same as in Fig. 2.

$$\sigma_{Ps} = \left(\frac{2}{k}\right)(2\pi)^3 \,\mathrm{Im}\langle \mathbf{k}0|W_{Ps}^{(Q)}|0\mathbf{k}\rangle. \tag{20}$$

III. Results

In the present calculation, 15 discrete states of hydrogen are included in P space. They are 1,2,3,4,5,6s, 2,3,4,5,6p, 3,4,5,6d. The optical potentials that describe the target continuum are in the couplings 1s-1s, 1s-2s, 2s-2s, 2p-2p, 1s-2p, 1s-3s, 3s-3s, 1s-3p, 3p-3p, 1s-3d, and 3d-3d. The optical potential that represents the formation of positronium in its $n=1$ and $n=2$ bound states is included in the coupling 1s-1s.

We display present ionization cross sections, in Fig. 1, comparing with experimental measurements and other theoretical results. The agreement of the present ionization cross section with experimental data of Jones *et al.* [12] is good. Experimental and theoretical ionization cross sections attain their maximum value at the same energy and decrease very

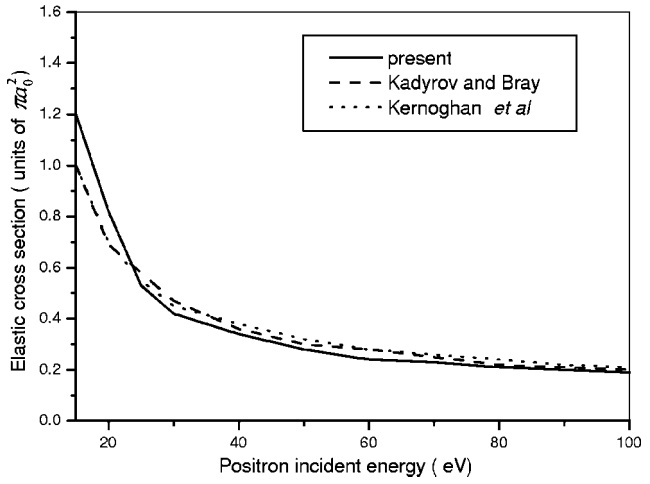

FIG. 4. Elastic cross section for positron scattering by hydrogen (πa_0^2). The notations are the same as in Fig. 2.

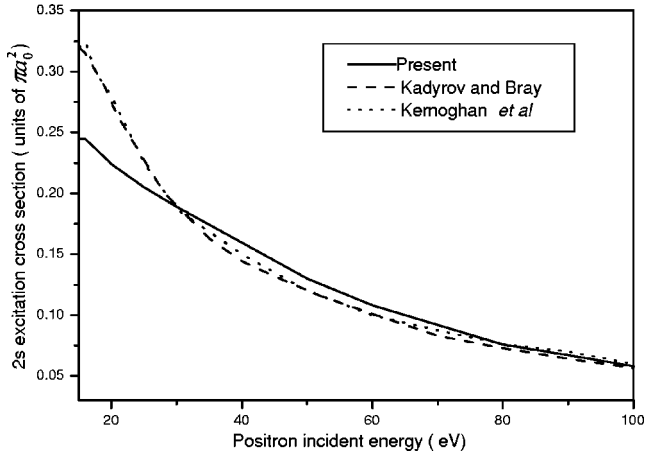

FIG. 5. 2*s* excitation cross section for positron scattering by hydrogen (πa_0^2). The notations are the same as in Fig. 2.

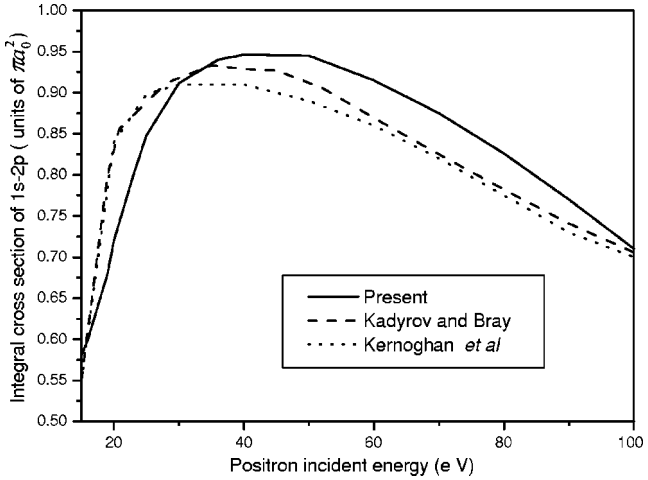

FIG. 6. 2*p* excitation cross section for positron scattering by hydrogen (πa_0^2). The notations are the same as in Fig. 2.

slowly with the same shape. The ionization cross sections obtained from different L^2 calculations (Mitroy [2], Kernoghan *et al.* [3], and Kadyrov and Bray [5]) have different values. The model with 28 pseudostates (Mitroy [2]) is very close to the experimental data except for a pronounced peak near 5 Ryd, while the ionization cross section is given by Kernoghan *et al.* [3] and convergent close-coupling approach (Kadyrov and Bray [5]) are higher than our ionization cross section and experimental data in the energy region 15–100 eV. It is probable that the ionization cross section obtained by L^2 pseudostates depends on the size of the L^2 basis and the values of l used for these orbitals.

The present cross section for positronium formation in $n=1$ and $n=2$ states is illustrated in Fig. 2, comparing with experimental data for positronium formation in all states and with the results of different close-coupling calculations. The present calculations are in good agreement with experimental measurements (Zhou *et al.* [4]). The positronium formation cross sections of Kernoghan *et al.* [3] and Mitroy [2] are higher than the present values, this is mainly because they have included $n>3$ positronium bound states by scaling their Ps cross section using the $(1/n)^3$ scaling rule (Mitroy [2]). It is very encouraging that the Ps potential in the present CCO approximation can depict the interaction of the positron and electron well. The quality of this method is being tested on other atoms.

The total cross section includes all contributions from accessible channels. It provides an overall check for a positron-atom scattering theory. The present CCO results for the total cross section are shown in Fig. 3, comparing with experimental data (Zhou *et al.* [4]) and other theoretical calculation results. The present total cross sections are in good agreement with experimental measurements in the energy region 15–100 eV. At higher intermediate energies the positronium formation cross section decreases very rapidly and contributes only a very small part to the total cross section. The

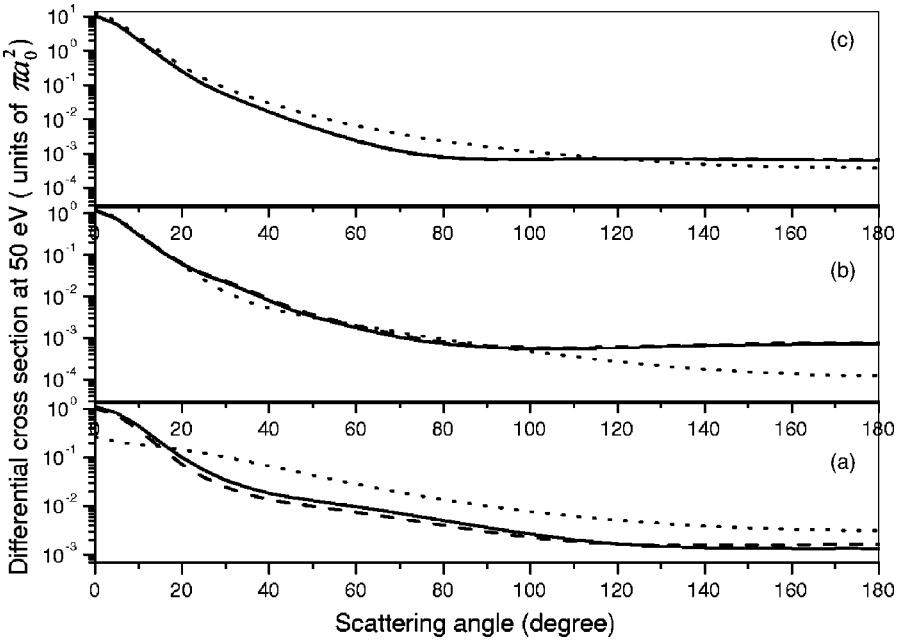

FIG. 7. Differential cross section of positron scattering by hydrogen at 15 eV (πa_0^2). For (a) elastic scattering, (b) 2*s* excitation, and (c) 2*p* excitation: the full curve, full optical potential results (continuum optical potential with positronium formation optical potential); dashed curve, continuum optical potential calculation only; dotted curve, pure close coupling calculation results.

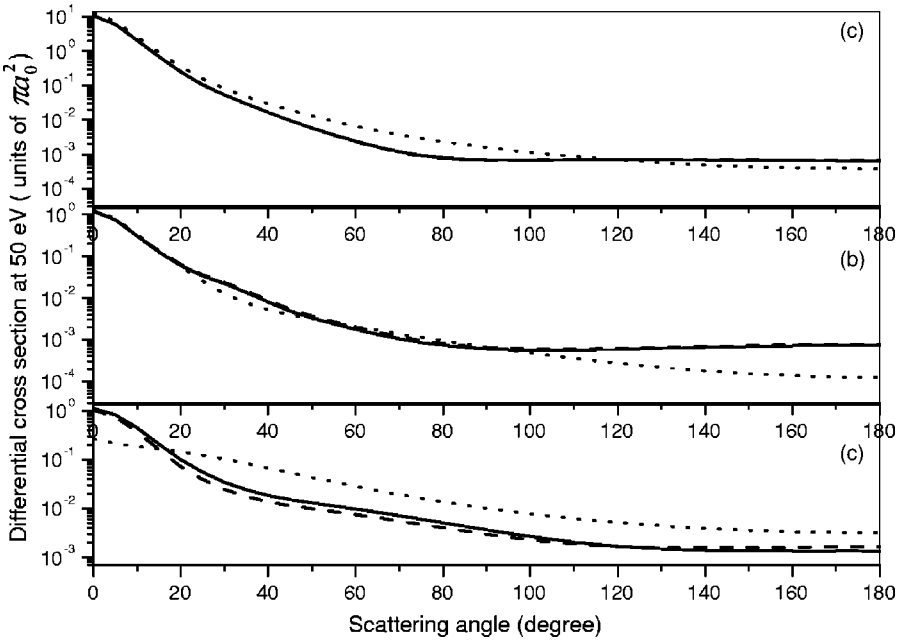

FIG. 8. Differential cross section of positron scattering by hydrogen at 50 eV (πa_0^2). The notations are the same as in Fig. 7.

ionization cross section plays a more important role at the higher energies and the contribution of higher bound states of positronium is negligible.

We display our calculations for cross sections of elastic scattering, 2*s* and 2*p* excitation in Fig. 4, Fig. 5, and Fig. 6. In the case of elastic scattering, the present integral cross sections are larger than both those of Kernoghan *et al.* [3] and those obtained by using the convergent close-coupling approach of Kadyrov and Bray [5] when impact energy $E<25$ eV, and very close to both of calculation results when $E>25$ eV. However the present integral cross sections of 2*s* excitation are smaller than both calculations of Kernoghan *et al.* [3] and convergent close-coupling approach (Kadyrov and Bray [5]) under 30 eV and also are very close to their data above 30 eV. For the integral cross sections of 2*p* excitation, we found that the present calculation results are smaller than both calculations of Kernoghan *et al.* [3] and convergent close-coupling approach (Kadyrov and Bray [5]) under positron incident energy 30 eV and are larger than their results above 30 eV. Probably, these differences in integral cross sections are due to different treatments of ionization continuum and positronium formation in calculations of present and the two center close-coupling methods. We also demonstrate the elastic and excitation differential cross sections of 2*s* and 2*p* at 15, 50, and 100 eV in Fig. 7, Fig. 8, and Fig. 9 with pure close coupling, continuum optical potential and full optical potential (ionization continuum with positronium formation optical potential) calculations, respectively. Comparisons show that positronium formation and continuum potentials produce significant effects upon the elastic and excitation differential cross sections and the effects are decreasing as positron incident energy is increasing.

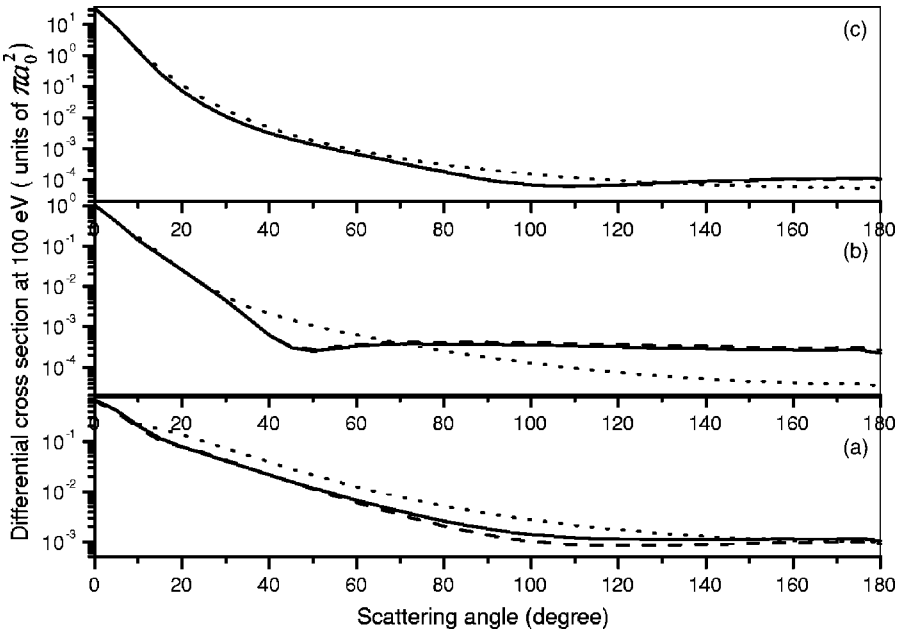

FIG. 9. Differential cross section of positron scattering by hydrogen at 100 eV (πa_0^2). The notations are the same as in Fig. 7.

IV. CONCLUSIONS

We have performed that coupled channels optical calculations for positron scattering by hydrogen at intermediate energies 15–100 eV. We solve coupled integral equations to convergence for discrete physical channels in P space and have developed an equivalent-local complex optical potential to describe the interaction of the projectile with the target, various physical mechanisms in positron-atom scattering. The real part of the potential describes virtually excitation of the target continuum and virtual formation of positronium, the imaginary part describes real excitation of these channels and the formation of positronium bound states. Satisfactory agreements with experimental measurements (Zhou *et al.* [4]) have been achieved. We also calculated integral cross sections and differential cross sections for elastic and excitation cross sections of $2s$ and $2p$. Calculated results demonstrated that the coupled channels optical method has some virtues as a tool to study positron scattering by atoms. Application of the method to positron multielectron atom systems is straightforward.

ACKNOWLEDGMENTS

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