Elastic and inelastic positron–helium scattering*

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Elastic and inelastic positron–helium scatterings have been investigated with the coupled-channel optical method (CCO). Ionization continuum and positronium formation channels are included via a complex equivalent-local optical potential. Calculations are reported of cross sections of elastic scattering, total excitation and $n = 2$, 3, and 4 excitations of ground-state helium for incident energies from 30 eV to 400 eV. The present calculation shows that the ionization and Ps-formation channels significantly affect the cross sections of elastic and inelastic positron–helium scatterings.

Keywords: positron, helium, elastic scattering, excitation

PACC: 3485

1. Introduction

For years positron–atom scattering has been an important area of intense research in atomic and molecular physics since it can offer a new way to test our understanding of basic interaction in many-body systems in comparison with those provided by electrons, and it also has extensive applications in many areas such as plasma physics and materials science.[1−3] The study of elastic scattering and target excitations in positron scattering by light atoms is thus of great interest to both theoreticians and experimentalists. If the basic dynamical ingredients of the description for such a collision process can be identified, one can extend the analysis to more complicated systems. As helium is the simplest many-electron atom and an ideal target atom due to its stability, several experimental measurements and a number of theoretical studies of transition processes in positron–helium collision have been performed in the past decades.

Due to the technical restrictions, the experimental efforts on elastic positron–helium scattering and target excitations are limited; only the total excitation cross sections have been measured by Coleman *et al.*[4] and Mori and Sueoka.[5] Both groups used the time-of-flight (TOF) technique to obtain the cross sections. A problem with this method is its inability to distinguish between energy loss and angular deflection, which means that it cannot uniquely identify particular transitions. More detailed measurements demand new progress of positron-beam technology.

Besides both experimental measurements, there are a number of theoretical studies on elastic and inelastic positron–helium scatterings. Earlier distorted-wave (DW) calculations (DWC) have been made by Campeanu *et al.*,[6] Katiyar *et al.*,[7] and Parcell *et al.*[8,9] Their results show that the DWC results are sensitive to the exact form of the distortion potential, and these previous calculations exhibit large differences in the results predicted for scattering energies below 150 eV. In recent years, new progress in theoretical studies has been made in the applications of various close-coupling methods.[10−17] Both the ionization and rearrangement channels were included in the calculations by Hewitt *et al.*,[15] Campbell *et al.*[16] and Wu *et al.*[17] with the pseudo-state expansion. The target states are obtained by diagonalizing the target Hamiltonian in different basis. Hewitt *et al.*,[15] as well as Campbell *et al.*,[16] employed the basis of Slater-type orbitals (STO); the Ps-formation channels are taken into account by adding positronium bound states. The two calculations produced significantly larger cross sections. In the convergent close-coupling (CCC) calculation of Wu *et al.*,[17] the target states are obtained in the square-integrable orthogonal Laguerre basis and the positive-energy states account for both ionization and Ps-formation channels.

In this paper, we report a detailed study on the elastic and inelastic positron–helium scatterings

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and investigate the effect of ionization and rearrangement channels on various transitions with the coupled-channel optical method (CCO), in which a complex equivalent local potential is developed to include positronium formation channels. In a previous work,[18] we have applied this method to positron–helium scattering, the ionization, Ps-formation and total scattering cross section are reported above the Ps-formation threshold, and good agreement has been achieved with experimental and theoretical data.

We present a brief account of the theoretical model in Section 2. The results obtained for elastic scattering, target excitations and total excitation cross sections are reported from 30 eV to 400 eV in Section 3, and the conclusions are given in Section 4.

2. Model and method

The details of the CCO method for positron–helium scattering have been reported in our previous work.[18] Here we only briefly review the essential features.

We start the calculation by solving the momentum-space coupled-channel optical equation

$$\begin{aligned}&\langle \boldsymbol{k}, \Phi_i|T|\Phi_0, \boldsymbol{k}_0\rangle \\ =\ &\langle \boldsymbol{k}, \Phi_i|V^{(\mathrm{Q})}|\Phi_0, \boldsymbol{k}_0\rangle \\ &+ \sum_{j\in P}\int d^3\boldsymbol{k}'\langle \boldsymbol{k}, \Phi_i|V^{(\mathrm{Q})}|\Phi_j, \boldsymbol{k}'\rangle \\ &\times \frac{1}{E^+ - \epsilon_j - \frac{1}{2}k'^2}\langle \boldsymbol{k}', \Phi_j|T|\Phi_0, \boldsymbol{k}_0\rangle. \end{aligned} \quad (1)$$

The optical potential $V^{(\mathrm{Q})}$ can be expressed as the sum of the channel-coupling potential V and a nonlocal complex polarisation potential $W^{(\mathrm{Q})}$, where

$$W^{(\mathrm{Q})} = W_{\mathrm{I}}^{(\mathrm{Q})} + W_{\mathrm{Ps}}^{(\mathrm{Q})}. \quad (2)$$

Here $W_{\mathrm{I}}^{(\mathrm{Q})}$ and $W_{\mathrm{Ps}}^{(\mathrm{Q})}$ stand for the parts of the polarization potential that describe the ionization continuum and positronium formation process respectively. By using the weak-coupling approximation, the matrix element of the polarization potential can be written as

$$\begin{aligned}&\langle \boldsymbol{k}' i|W^{(\mathrm{Q})}|j\boldsymbol{k}\rangle \\ =\ &\sum_{n\in Q}\langle \boldsymbol{k}' i|V|\Psi_n^{(-)}\rangle \frac{1}{E^{(+)} - E_n}\langle \Psi_n^{(-)}|V|j\boldsymbol{k}\rangle, \end{aligned} \quad (3)$$

where $\Psi_n^{(-)}$ represents the time reverse of the exact state vector for a reaction starting in channel n. The notation n is a discrete notation for the three-body ionization continuum or the two-body positronium formation channels. Spin dependence is implicit in the notation.

The optical potential matrix element for positronium formation is:

$$\begin{aligned}&\langle \boldsymbol{k}' i|W_{\mathrm{Ps}}^{(\mathrm{Q})}|j\boldsymbol{k}\rangle \\ =\ &\sum_n \langle \boldsymbol{k}' i|V|\tilde{\chi}_n^{(-)}\rangle \frac{1}{E^{(+)} - E_n}\langle \tilde{\chi}_n^{(-)}|V|j\boldsymbol{k}\rangle, \end{aligned} \quad (4)$$

$$\begin{aligned}&|\tilde{\chi}_n^{(-)}\rangle \\ =\ &(1 - |\psi_i\rangle\langle\psi_i|)|\Psi_n^{(-)}\rangle, \end{aligned} \quad (5)$$

$|\tilde{\chi}_n^{(-)}\rangle$ is orthogonalized to the ground state of helium $|\psi_i\rangle$, from which the electron is captured, and

$$(\varepsilon_j - H_{\mathrm{T}})|\psi_i\rangle = 0. \quad (6)$$

Here, H_{T} is the target Hamiltonian. The independent-particle model has been used for calculating the potential matrix element.

For computation, a partial-wave expansion of the T-matrix and V-matrix elements is performed.[19] It is

$$\begin{aligned}&\langle \boldsymbol{k}' i|T|j\boldsymbol{k}\rangle \\ =\ &\sum_{L,M,N,L',M',N'J,K,S,N_S} \\ &\times \langle \hat{\boldsymbol{k}}|L', M'\rangle C_{L'l'J}^{M'm'K} C_{\frac{1}{2}s'S}^{n'N'N_S} T_{I'I}^{JS}(k, k') \\ &\times C_{LlJ}^{MmK} C_{\frac{1}{2}sS}^{nNN_S} \langle L, M|\hat{\boldsymbol{k}}'\rangle, \end{aligned} \quad (7)$$

where

$$\langle \hat{\boldsymbol{k}}|L, M\rangle \equiv Y_{LM}(\hat{\boldsymbol{k}}). \quad (8)$$

C_{LlJ}^{MmK} is a Clebsch–Gordan coefficient. The index I is the L-channel index. $L, M, \frac{1}{2}, N$ represent the partial-wave orbital and spin angular momentum. J, K, S, N_S represent the orbital and spin angular momentum of the channel state. Orbital and spin angular momentum and their projections for the target state are represented by l, m, s, n. Then the total cross section can be written as

$$\begin{aligned}\sigma_{ij} =\ &(2\pi)^4 \frac{k'}{k}\frac{2S+1}{2(2s+1)(2l+1)} \\ &\times \frac{1}{4\pi}\sum_{L,L',J}(2J+1)|T_{I'I}^{JS}|^2. \end{aligned} \quad (9)$$

3. Results and discussions

The present calculation results are reported and compared with available theoretical and experimental data in this section. We have also given the calculations with and without the optical potentials responsible for the ionization continuum and Ps-formation

channels, namely CCOB and CCOA, to distinguish the effects of these channels. The target bound states are represented by configuration interaction (CI) wave functions. The basis used in the CI representation consists of all allowed excitations of electrons in the 1, 2, 3, 4s; 2, 3, 4p; 3, 4d states and the pseudo-orbital $\overline{\mathrm{s}}, \overline{\mathrm{p}}, \overline{\mathrm{d}}$.[20]

3.1. Elastic scattering and He(2^1S, 2^1P) excitation

The cross sections for elastic scattering and He(2^1S, 2^1P) excitation calculated using the current models are displayed in Figs. 1, 2 and 3 respectively. The calculations of Campeanu *et al.*,[6] Hewitt *et al.*,[15] Campbell *et al.*,[16] and Wu *et al.*[17] are also presented for comparison. The results of these transitions exhibit a similar trend that all the theoretical calculations have a similar energy dependence but are significantly different in magnitude, especially in the lower energy region. The calculations of Hewitt *et al.*[15] and Campbell *et al.*[16] yield significantly larger cross sections, while the present CCOB calculation usually shows better agreement with the DW calculation of Campeanu *et al.*[6] and CCC calculation of Wu *et al.*[17] except the discrepancies at lower energies in He(2^1S) excitation. The obvious discrepancies between different theoretical studies at lower energies is mainly due to the different treatments of ionization and Ps-formation channels that are expected to play an important role in this energy region.

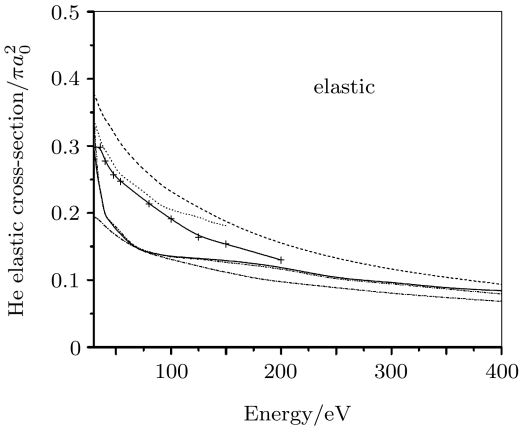


Fig. 1. The elastic cross section of positron–helium scattering as a function of energy E. A comparison between the present CCOB (solid), present CCOA (dashed), and the results of Campeanu *et al.*[6] (dot-dot-dashed), Hewitt *et al.*[15] (solid with symbols +), Campbell *et al.*[16] (dotted), and Wu *et al.*[17] (dot-dashed) is shown.

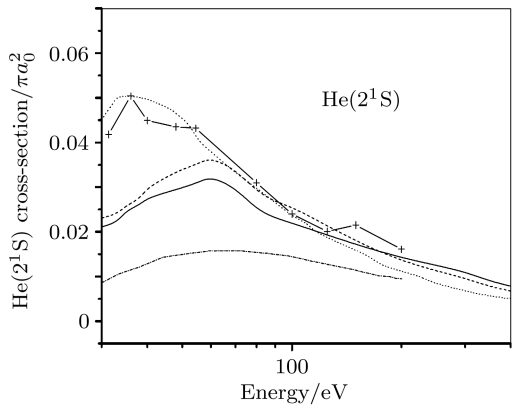


Fig. 2. He(2^1S) excitation cross section as a function of energy E. A comparison between the present CCOB (solid), present CCOA (dashed), and the results of Hewitt *et al.*[15] (solid with symbols +), Campeanu *et al.*[6] and Parcell *et al.*[8] (dot-dashed), and Wu *et al.*[17] (dotted) is shown.

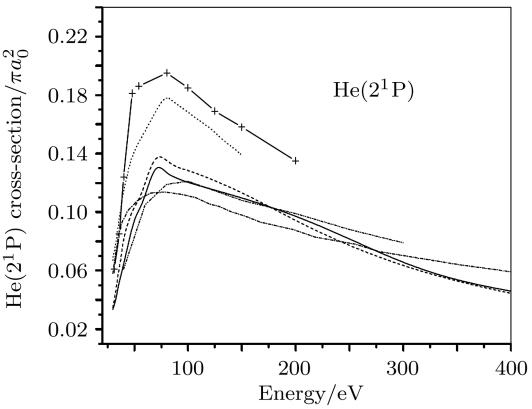


Fig. 3. He(2^1P) excitation cross section as a function of energy E. A comparison between the present CCOB (solid), present CCOA (dashed), and the results of Campeanu *et al.*[6] (dot-dot-dashed), Hewitt *et al.*[15] (solid with symbols +), Campbell *et al.*[16] (dotted), and Wu *et al.*[17] (dot-dashed) is shown.

The comparison between the present CCOA and CCOB results is also displayed to see the effect of ionization and Ps-formation channels. In Fig. 1, the large difference between CCOA and CCOB results indicates that the inclusion of ionization and Ps-formation channels significantly reduces the elastic cross sections. For He(2^1S) excitation, good agreement has been achieved above 100 eV (see Fig. 2), which shows that the ionization and Ps-formation channels have little significance in this energy region. Below this energy, the effect of these channels is to reduce the cross sections. In Fig. 3, the inclusion of ionization and Ps-formation channels slightly lowers the cross sections up to 150 eV. It is obvious that the largest effect of ionization and Ps-formation channels occurs at lower energies and is always to reduce the cross sections for elastic scattering and He(2^1S) and He(2^1P) excitation.

3.2. He($n = 3, 4$) excitation

The cross sections for He ($n = 3, 4$) transitions are shown in Figs. 4 and 5, along with the DW calculation of Campeanu *et al.*[6] and Katiyar *et al.*[7] Figure 4 shows the present cross sections for He($n = 3$) excitations. The excitation to the 3^1P state is more important. Its cross section is three times larger than the results of 3^1S and 3^1D states in the present calculation. For He(3^1P) excitation, although the calculation of Katiyar *et al.*[7] produces higher values and different energy dependence, the agreement between the present calculation and the results of Campeanu *et al.*[6] is good, except for the discrepancy in the peak position, which is 100 eV and 75 eV respectively. In the cross sections for He ($n = 4$) excitations in Fig. 5, the present calculation of He(4^1P) excitation predicts lower values than those of Campeanu *et al.*;[6] however, they have similar energy dependence.

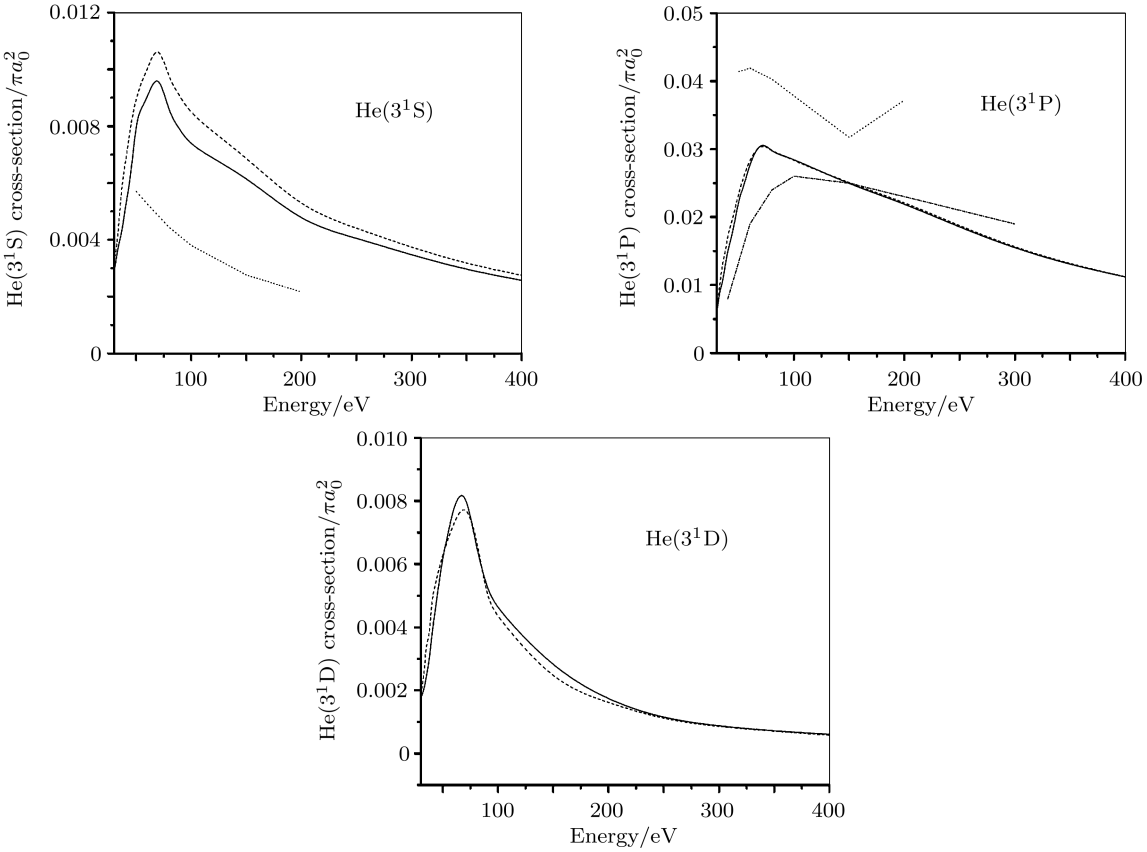
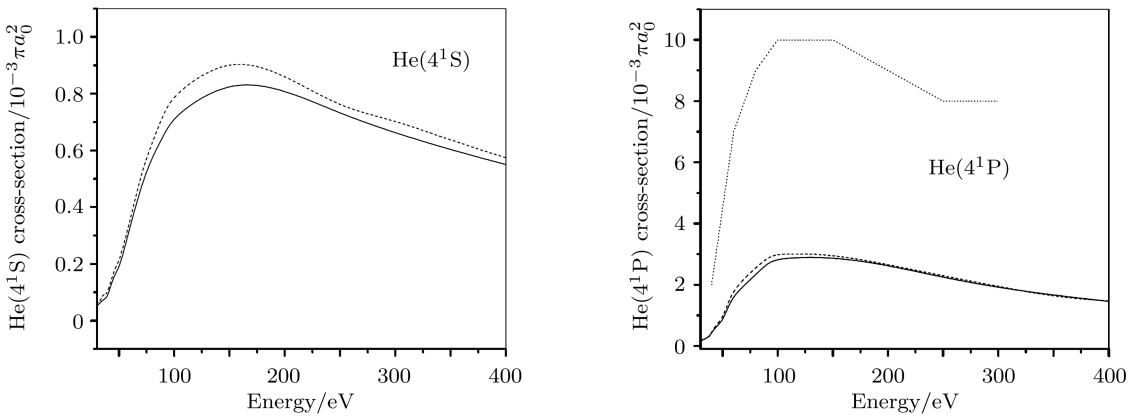


Fig. 4. He ($n = 3$) excitation cross section as a function of energy E. The results of the present CCOB (solid), CCOA (dashed), Katiyar *et al.*[7] (dotted), and Campeanu *et al.*[6] (dot-dashed) are displayed.



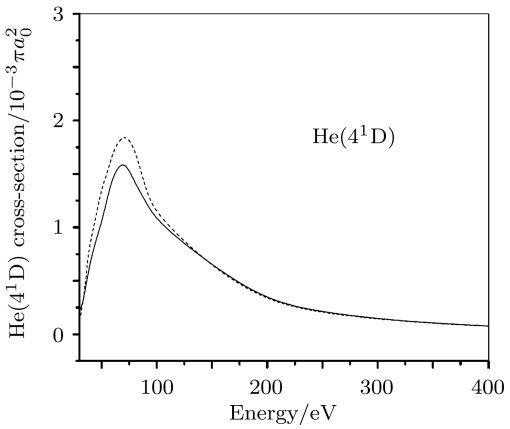


Fig. 5. He ($n = 4$) excitation cross sections. The results of the present CCOB (solid), CCOA (dashed), and Campeanu *et al.*[6] (dotted) are displayed.

From the comparison in Figs. 4 and 5, the effect of the ionization and rearrangement channels in $n = 3, 4$ transitions is different from the case for elastic scattering and He(2^1S) and He(2^1P) excitations. For the excitations of 3^1S, 4^1S, 4^1D states, the inclusion of these channels reduces the cross sections at lower energies, especially around the peak position, as we have seen in elastic scattering and He(2^1S) and He(2^1P) excitations, while it is negligible for the 3^1P, 3^1D, 4^1P excitations.

3.3. Total excitation

To gain a better insight into the target excitation process of positron–helium collision, a new partition of total excitation cross sections is displayed in Fig. 6. Here the dotted line and the dot-dashed line are the sums of cross sections for He($n = 3$) and He($n = 4$) excitations respectively. From this figure, the dominance of the contribution of the transition to the 2^1P state is evident, and we can also find that the contribution of excitations of $n = 3$ states is larger than that expected in the present calculation.

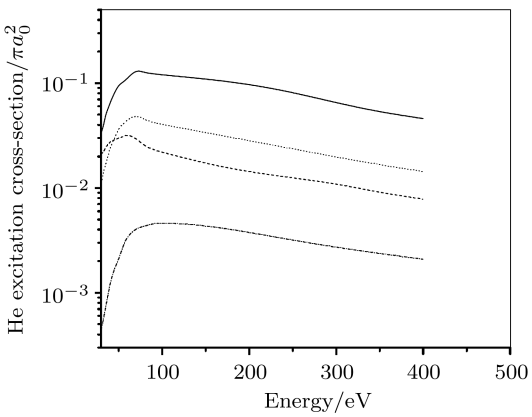


Fig. 6. Present partition of total excitation cross sections. The cross sections of 2^1S (dashed), 2^1P (solid), He($n = 3$) (dotted) and He($n = 4$) (dot-dashed) excitations are presented.

The total excitation cross sections are shown in Fig. 7, along with the measurement of Mori and Sueoka[5] and close-coupling calculations of Hewitt *et al.*[15] and Wu *et al.*,[17] while these theoretical results are all calculated as the sum of 2^1S, 2^1P excitations. In the measurement of Mori and Sueoka,[5] the separation of contribution from excitation is also based on the theoretical data for 2^1S+2^1P excitations of Parcell *et al.*;[8,9] we thus display the relevant CCOB results in Fig. 7. The CCOB 2^1S+2^1P cross section shows better agreement with the experimental data, while the other calculations overestimate the measurements.

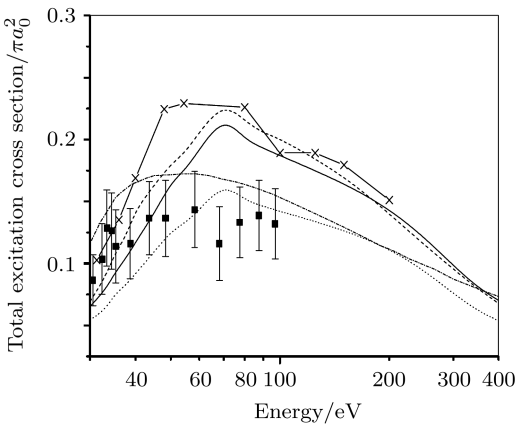


Fig. 7. Total excitation cross section as a function of energy E. A comparison between the present CCOB (solid), present CCOA (dashed), CCOB 2^1S+2^1P (dotted), and the results of Hewitt *et al.*[15] (solid with symbols ×), Wu *et al.*[17] (dot-dashed), and the measurements of Mori and Sueoka[5] (black square) is shown.

The largest discrepancy between different calculations occurs in the peak position, which is around 70 eV for Hewitt *et al.*[15] and the present results, and about 45 eV for the other studies. The fact that the present 2^1S+2^1P cross section is obviously lower than the total excitation cross section indicates that $n \geq 2$ transitions have non-negligible contributions in the present calculation. The comparison between present CCOA and CCOB results shows that the inclusion of ionization and Ps-formation channels reduces the cross sections below 150 eV.

4. Conclusions

A detailed study of various transitions in positron scattering with ground-state helium has been performed using the CCO method, in which the ionization and Ps-formation channels are included via an equivalent local potential. The cross sections of elastic scattering and target excitations of $n = 2, 3, 4$ states are reported for incident energies from 30 eV to 400 eV. The present calculation shows that the inclusion of ionization and Ps-formation channels has a significant effect on the elastic and inelastic positron–helium scattering, which always reduces the cross sections at lower energies. Given the evident differences between different theoretical studies, the present results show good agreement with the calculations of Campeanu *et al.*[6] and Wu *et al.*[17] except for the discrepancies at lower energies. The present total excitation cross sections agree well with the experimental data. Unfortunately, there are no experimental measurements for particular transitions. More experimental and theoretical research is desired.

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