Convergent close-coupling calculations of positron-magnesium scattering

Jeremy S. Savage,* Dmitry V. Fursa, and Igor Bray
ARC Centre for Antimatter-Matter Studies, Curtin University of Technology, GPO Box U1987, Perth, WA 6845, Australia
(Received 11 May 2011; published 21 June 2011)

The single-center convergent close-coupling method has been applied to positron-magnesium scattering at incident energies from 0.01 to 100 eV. Cross sections are presented for elastic scattering and excitation of $3\,^1P$, as well as for the total ionization and total scattering processes. We also provide an estimate of the positronium formation cross section. The results agree very well with the measurements of the total cross section by Stein *et al.* [Nucl. Instrum. Methods Phys. Res. Sect. B **143**, 68 (1998)], and consistent with the positronium formation measurements of Surdutovich *et al.* [Phys. Rev. A **68**, 022709 (2003)] for positron energies above the ionization threshold. For energies below the positronium formation threshold (0.8 eV) we find a large P-wave resonance at 0.17 eV. A similar resonance behavior was found by Mitroy and Bromley [Phys. Rev. Lett. **98**, 173001 (2007)] at an energy of 0.1 eV.

DOI: 10.1103/PhysRevA.83.062709 PACS number(s): 34.80.Uv, 34.80.Bm, 34.80.Dp

I. INTRODUCTION

There have been significant recent advancements in both the experimental and theoretical treatment of positron interactions with atoms, though the field still remains less developed than in the case of electron-atom scattering [1]. The difficulty of obtaining low energy, monochromatic positron sources has been limiting progress from the experimental side. The theory is also less developed due to the two-center nature of the problem requiring considerable computational resources. Furthermore, some conceptual challenges still remain.

The scattering problem of positrons is somewhat similar to that of electrons, and superficially might even look simpler as complications associated with the Pauli exclusion principle do not apply. As with electrons, positron collisions lead to elastic scattering, target excitation, and ionization. In place of the exchange channels, positron scattering has channels known as positronium (Ps) formation, where the incident positron captures an atomic electron to form a positronium atom. Account of the positronium formation channels, whose center of mass is away from the atom, represents a major difficulty in the theoretical treatment of positron collisions with atoms and molecules.

The "exotic" Ps atom has a ground state energy of -6.8 eV, and hence Ps formation opens at IP-6.8 eV, where IP is the first ionization potential of the target. For magnesium IP is 7.6 eV, and thus the Ps-formation threshold is 0.8 eV. This makes magnesium an interesting positron scattering target as very few elements have such a low yet positive threshold. In comparison, the most studied targets, hydrogen and helium, have Ps-formation thresholds of 6.8 and 17.8 eV, respectively. Others, such as the alkali metals, have negative thresholds, that is, the Ps-formation channel is open at all incident positron energies.

Considerably less experimental data exist for positron-magnesium scattering than for the electron case. To date, the only available data are due to the "Detroit group" at Wayne State University [2–4] who have measured the total cross sections, as well as the upper and lower limits for Ps-formation cross sections. They noted many difficulties associated with use of the magnesium target and as such regard their latest values as "preliminary" [2]. Unfortunately their measurements did not extend to incident energies below the Ps-formation threshold which proved to be of interest, particularly in relation to the existence of bound states of the Mg-e^+ system.

Calculations of positron-magnesium scattering are more numerous. The polarized orbital method (POM) was used by Szmytkowski [5] to calculate elastic scattering cross sections. However, they proved to be in poor agreement with the experiment. Campeanu *et al.* [6] combined a POM-calculated elastic cross section with an inelastic cross section, calculated using a distorted wave approximation (DWA), to give total cross sections at intermediate and high energies. Their results agree with the experimental data above 30 eV, but significantly underestimate the experiment at lower energies.

Elastic cross sections, phase shifts, and scattering lengths were calculated by Bromley *et al.* [7] using a polarized orbital model by tuning the free parameters to replicate the positron bound energy (0.373 eV). The latter was obtained using the stochastic variational principle [8]. We note that analysis of low-energy behavior of s-wave phase shifts in previous calculations of positron-magnesium scattering have predicted the bound Mg-e^+ state. However, the binding energy varied widely depending on the calculation details (see Table 1 in Bromley *et al.* [7]).

The positronium formation channels were explicitly accounted for by Hewitt *et al.* [9] who performed two-center close-coupling calculations (CCA). These calculations include two states of Mg ($3s^2\,^1S^e$, $3s3p\,^1P^o$) and three states of positronium Ps($1s$), Ps($2s$), Ps($2p$). Cross sections for all of the states present in the close-coupling expansion have been obtained, but when summed to obtain the total cross section the agreement with experiment of Stein *et al.* [2] proved to be poor.

Gribakin and King [10] used many-body theory methods to calculate phase shifts and total cross sections. Their calculations accounted for the Ps-formation channels and demonstrated their significant effect on the cross sections. However, their results did not agree with experiment [4]. An

*jeremy.savage@student.curtin.edu.au

interesting feature of the Gribakin and King calculations is the prediction of a bound Mg-e$^+$ state in the s wave with 0.985 eV binding energy and in the p wave with 0.159 eV binding energy as well as a shape resonance in the d wave at 1 eV. Note that the binding energy of the s-wave bound state they obtained differed substantially from the prediction of the stochastic variational principle [8]. Bromley *et al.* [7] suggested that difficulties in the calculation of the correlation potential by Gribakin and King [10] were probably the reason for the disagreement.

More recently Mitroy *et al.* [11,12] used a novel technique to investigate low-energy positron-magnesium scattering. In this technique the semiempirical optical potential has been tuned using a large configuration interaction (CI) calculation. While positronium formation channels have not been included explicitly in the calculation they have been accounted for indirectly via the large CI expansion. Phase shifts and elastic cross sections were calculated. Interestingly, contrary to the results of Gribakin and King [10], a prominent p-wave shape resonance was predicted at positron energies of approximately 0.1 eV while no resonance behavior was found for d-wave scattering.

The purpose of this paper is to investigate positron-magnesium scattering using the convergent close-coupling (CCC) method in the single-center formulation. The CCC method has been extensively tested for electron-atom scattering [13,14] including scattering from alkaline-earth atoms [15–18]. It was also applied successfully (in a single center mode) to positron scattering from H [19], He [20], and noble gases [21,22]. Note that, while a two-center CCC method has been recently developed for helium [23], application to magnesium is a major extension to be completed some time in the future.

In the single-center CCC method the change from an incident electron to a positron requires a simple change of sign of the projectile charge and dropping the projectile-atom exchange with no further changes to the computer code. Conceptually the method is particularly simple. However, computationally the problem becomes very different to electron-atom scattering. The positronium formation channels are not accounted for explicitly, but are included indirectly via unusually large close-coupling expansions that include a large number of positive-energy pseudostates of high orbital angular momentum l. For incident positron energies above the target atom ionization threshold the total ionization cross section (TICS) obtained in the CCC method provides an accurate estimate of the sum of direct ionization and positronium formation. In the low-energy region where positronium formation channels are closed the CCC method can again provide an accurate estimate of elastic scattering cross sections. In this case virtual Ps-formation channels, which play a vital role in the scattering, are also taken into account. The incident energy region between the positronium formation threshold and the ionization threshold still proves to be problematic. At these energies the positronium formation channels are open but the positive energy pseudostates that model the breakup are closed. As a result a lack of convergence is found on this small energy range.

The paper is organized as follows. In the next section we present the details of CCC method specific to positron scattering from magnesium. In Sec. III we present our results and compare with experiment and other calculations. Conclusions are formulated in Sec. IV.

II. THEORY

We model Mg as a system with two active electrons above a frozen Hartree-Fock core [15,17]. A set of one-electron orbitals $\{\varphi_{nl}\}$ is obtained via diagonalization of the Mg$^+$ Hamiltonian in a Sturmian (Laguerre) basis,

$$\xi_{nl}(r) = \sqrt{\frac{\lambda_l (n-1)!}{(2l+1+n)!}} (\lambda_l r)^{l+1} \exp(-\lambda_l r/2) L_{n-1}^{2l+2}(\lambda_l r), \tag{1}$$

where λ_l are exponential fall-off parameters and

$$L_{n-1}^{2l+2}(x) = \sum_{m=0}^{j} \frac{(-1)^m (j+n)!}{(j-m)!(n+m)!m!} x^m \tag{2}$$

are the associated Laguerre polynomials, l is the angular momentum and n ranges from 1 to the basis size N_l. The exponential fall-off parameters were chosen to be $\lambda_l = 3.0$. The number of one-electron orbitals N_l for given value of angular momentum l was chosen to be $N_l = 18$ for $l = 0, \ldots, 6$ and $N_l = 24 - l$ for $l = 7, \ldots, l_{\max}$ with $l_{\max} = 20$. Such a choice was made as a result of convergence studies as discussed later in the paper. The maximum value of angular momentum $l_{\max}$ will ultimately determine the size $N = \sum_{l=0}^{l_{\max}} N_l$ of the scattering calculations, and will also be a subject of the convergence studies. Note that in electron-scattering typically $l_{\max} = 5$ suffices.

The one-electron orbitals $\{\varphi_{nl}\}$ are used to form a set of antisymmetric two-electron configurations, followed by standard CI calculations of the Mg wave functions. The calculated Mg states $\{\phi_f^N\}$, $f = 1, \ldots, N$, diagonalize the Mg target Hamiltonian H_{T},

$$\langle \phi_f^{(N)} | H_{\mathrm{T}} | \phi_i^{(N)} \rangle = \epsilon_f^{(N)} \delta_{fi}, \tag{3}$$

where ϵ_f are the (pseudo)state energies. The target (pseudo)states $\phi_f^{(N)}$ are expressed via two-electron configurations as

$$|\phi_f^{(N)}\rangle = \sum_{\alpha,\beta} C_{\alpha\beta}^f |\varphi_\alpha \varphi_\beta : L_f S_f\rangle, \tag{4}$$

where $\alpha \equiv nl$. The orbital and spin angular momenta are denoted by L_f and S_f, respectively. The lowest energy states are good approximations of the Mg bound eigenstates, whereas the higher energy pseudostates provide for a discretization of the target continuum.

The choice of two-electron configurations is important for accurate descriptions of the Mg wave functions. We adopted a set of configurations which consist of configurations of two types. First, we include all configurations that are allowed by the selection rules when active electrons occupy any of the first two of $l = 0$, 1, and 2 orbitals. Second, we include frozen-core configurations where the "outer" electron is allowed to occupy any of the one-electron orbitals, while the "inner" electron is limited to the $3s$ orbital only. Configurations of the first type include the short range electron-electron

correlations necessary particularly for the accurate description of the ground state of magnesium, while configurations of the second type allow for square-integrable discretization of the target continuum. Ultimately, the reason for such a choice of configurations is related to the need for the close-coupling expansion not be too large in order to make scattering calculations feasible. This model has a total of $N = 305$ states.

One-electron (V_1^p) and two-electron (V_2^p) polarization potentials can be used to account for the polarization of the inert Hartree-Fock core [15], via

$$V_1^p(\boldsymbol{r}_1) = -\frac{\alpha_d}{r^4} W_6(r_1/\rho_l), \tag{5}$$

$$V_2^p(\boldsymbol{r}_1,\boldsymbol{r}_2) = -\frac{\alpha_d}{r_1^3 r_2^3}(\boldsymbol{r}_1\cdot\boldsymbol{r}_2)\sqrt{W_6(r_1/\rho_d)W_6(r_2/\rho_d)}, \tag{6}$$

$$W_6(r/\rho) = 1 - e^{-(r/\rho)^6}, \tag{7}$$

where indices "1,2" refer to the Mg valence electrons. In the present calculations the one-electron core dipole polarizability of Mg^{++} and fall-off parameter were set to $\alpha_d = 0.48$ and $\rho_l = 1.4$, respectively, for all l while two-electron polarization potential was set to zero. This choice produces a sufficiently accurate description of the Mg target structure, yielding the $(3s^2)^1S$ ground state ionization energy of 7.63 eV (experimentally 7.65 eV). The $(3s3p)^1P^o$ excitation energy is 4.39 eV which compares well with the experimental excitation energy of 4.35 eV. The oscillator strengths (in a.u.) for the $(3s3p)^1P^o$–$(3s^2)^1S$ transition are $f_l = 1.75$ (length) and $f_v = 1.70$ (velocity). These agree well with each other as well as with the multiconfiguration Hartree-Fock calculations of Froese-Fischer [24], $f_l = 1.76$ and $f_v = 1.74$ and the recommended value of $f = 1.80$ [25]. The calculated static dipole polarizability of 71.0 also compares favorably with the recent theoretical estimate of 71.26 by Derevianko *et al.* [26].

Excitation energies could be improved further using l-dependent fall-off parameters in the one-electron polarization potential together with nonzero two-electron polarization potential. We chose not to do so for the sake of simplicity of the calculations and to keep any phenomenological part of the calculations to a minimum. The stability of the calculated cross sections with respect to the variation of the polarization potential parameters will be discussed in the next section.

The set of calculated Mg target states $\{\phi_{nl}^N\}$ comprises of negative energy states (relative to Mg^+ ground state) and positive energy states. In the CCC method the target state basis is used to perform a close-coupling expansion of the total wave function and formulate the coupled Lippmann-Schwinger equations for the T matrix,

$$\begin{aligned}\langle k_f\phi_f^{(N)}|T|\phi_i^{(N)}k_i\rangle &= \langle k_f\phi_f^{(N)}|V|\phi_i^{(N)}k_i\rangle \\ &+ \sum_{n=1}^{N}\int_o^\infty dk\,\frac{\langle k_f\phi_f^{(N)}|V|\phi_n^{(N)}k\rangle\langle k\phi_n^{(N)}|T|\phi_i^{(N)}k_i\rangle}{E+i0-\epsilon_n^{(N)}-k^2/2}.\end{aligned} \tag{8}$$

The potential V comprises the Coulomb interaction of the positron with the two valence electrons of Mg, and the Coulomb interaction with the Mg core. It also includes the model polarization potentials (5) and (6). The positron-Mg potential is the negative of the direct potential for electron-Mg scattering as detailed by Fursa and Bray [15]. The Lippmann-Schwinger equation (8) is solved in a standard manner [13,14] to obtain transition amplitudes $T_{fi}^{(N)}$, and hence the various cross sections. The total cross section is obtained as a sum over cross sections of all open states included in the close-coupling expansion, while the TICS is obtained as a sum over cross sections of all open positive-energy states. The convergence of the calculations can be simply tested by increasing the size of the close-coupling expansion (parameters N_l, $l_{\max}$).

In addition to the CCC calculations we have also performed close-coupling calculations that have only negative-energy states. These calculations, labeled CC, have three ^1S, ^1P, ^1D states, two ^1F states, and one ^1G and ^1H states. This model has static dipole polarizability $\alpha = 70.5$, practically the same as in the CCC model. The difference between the CCC and CC results should highlight the importance of coupling to ionization and positronium formation channels.

III. RESULTS AND DISCUSSION

A. Total cross section

Figure 1 shows a comparison of the total cross sections obtained in the CCC and CC calculations with the experimental data of Stein *et al.* [2], and theoretical calculations of Gribakin and King [10], Hewitt *et al.* [9], Campeanu *et al.* [6], Bromley *et al.* [7], and Mitroy *et al.* [12].

The CCC and CC calculations agree only at high energies. As the incident energy decreases they diverge with the CC results becoming progressively smaller. At low energies we see very different behavior of the CCC and CC cross sections. In the case of electron-atom scattering there is usually close agreement between the CCC and CC calculated TCS results, particularly below the ionization threshold. The remarkable difference between CCC and CC results for positron-magnesium scattering at low energies is, therefore, an

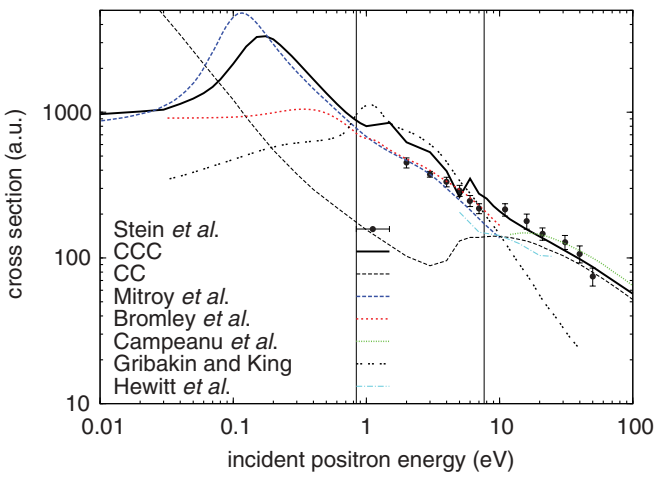

FIG. 1. (Color online) Total cross section for positron scattering on the ground state of magnesium. The present CCC and CC calculations are compared to the experimental data of Stein *et al.* (1998), and theoretical results of Mitroy *et al.* [12], Bromley *et al.* [7], Campeanu *et al.* [6], Gribakin and King [10], and Hewitt *et al.* [9]. The vertical lines indicate positronium formation (0.8 eV) and ionization (7.6 eV) thresholds.

indication of importance of coupling to positronium formation channels, even if they are closed.

For incident energies above the ionization threshold the CCC results agree very well with experiment. In the energy range between the positronium formation threshold and the ionization threshold the CCC results are not accurate. The reason for this is related to how the single-center CCC method models the positronium formation channels. In the CCC method the positronium formation channels are modeled via excitation of positive-energy pseudostates with large angular momentum and/or energy. In the 0.8–7.65 eV energy region all these pseudostates are closed while at least one positronium formation channel is open. The single-center model is therefore unphysical in this energy region and as a result cannot produce convergent results. Here, a two-center close-coupling approach to positron-magnesium scattering would be required to adequately describe the scattering processes. We note that the calculations of Bromley *et al.* [7] and Mitroy *et al.* [12] are in very good agreement with the experiment in this energy region.

At the very low-energy region (below 0.8 eV), where there is no experiment, we observe large differences between the various theoretical results. The calculation of Mitroy *et al.* [12] predicts a pronounced resonance behavior with a peak at 0.1 eV, while calculations of Bromley *et al.* [7] and Gribakin and King [10] do not. Somewhat like the results of Mitroy *et al.* [12], the CCC calculations predict a p-wave shape resonance with a cross section maximum at 0.17 eV. In Fig. 2 we compare s- and p-wave phase shifts with those of Mitroy *et al.* [12] (for the potential labeled V_{p2}). We find practically identical results for the s-wave phase shifts, however for the p wave we find substantial differences. The reason for the discrepancy in position of the p-wave resonance is unclear. Our calculation for the d-wave phase shift, also presented in Fig. 2, does not support the prediction of Gribakin and King [10] of a low-lying resonance at approximately 1 eV. While the incident energy of 1 eV is above the positronium formation threshold we find our single-center calculation stable up to 1.5 eV. The reason for such stability is related to the positronium formation cross section being relatively small in this energy region.

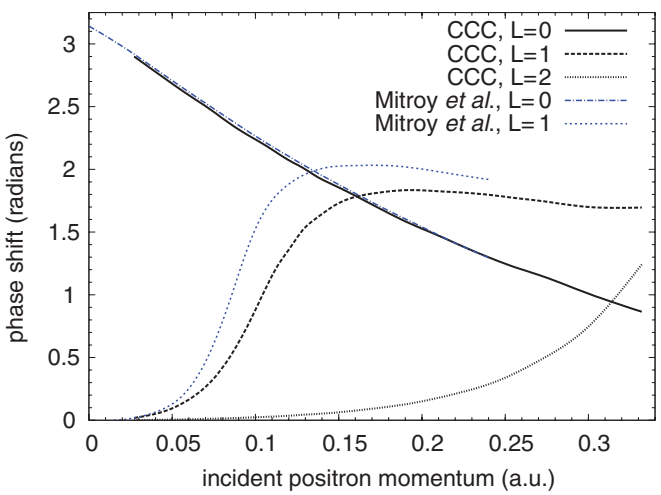

FIG. 2. (Color online) Positron-magnesium elastic phase shifts in the low-energy region.

B. Convergence of the CCC results

In order to verify the accuracy and convergence of the CCC calculations we performed a series of detailed convergence studies.

First, we have investigated the convergence of the calculated cross sections with respect to the accuracy of the Mg wave functions. The Mg ground state and low-lying excited states are most affected by electron-electron correlations. In our calculation these correlations are accounted for via two-electron configurations ($nln'l'$) that are built from one-electron orbitals satisfying: $l \leqslant l_a$ and $n - l \leqslant n_a$. The model described in the previous section for which we performed calculations includes all configurations that are allowed by the selection rules when active electrons occupy any of the first two of $l = 0,1$ and 2 orbitals, that is, $n_a = 2$ and $l_a = 2$.

In order to verify the convergence of our results with respect to the account of electron-electron correlations we have performed calculations for a number of models with different n_a and l_a values. Namely, we have performed calculations using a model with $n_a = 3$ and $l_a = 3$. This model has a marginally more accurate description of Mg wave functions, but it leads to a significantly larger close-coupling expansion. For this model the ground state ionization energy is 7.63 eV and the $(3s3p)^1P^o$ excitation energy of 4.38 eV. The oscillator strengths for the $(3s3p)^1P^o$–$(3s^2)^1S$ transition are $f_l = 1.75$ and $f_v = 1.71$ and the Mg static dipole polarizability is 71.2. We find that at energies above the Mg atom ionization threshold there is perfect agreement between the two models. Similarly, at the energies close to and below the positronium formation threshold there is very good agreement between the two models with only small differences (less than 5%) around the resonance maximum. The position and shape of the resonance proved to be well described by the smaller model ($n_a = 2$ and $l_a = 2$). Hence we have performed all further calculations in this model.

We investigated the stability of the cross sections with respect to the change in fall-off parameters of one- and two-electron polarization potentials. We found that our scattering calculations were insensitive to small variations of these parameters. For example, the choice of the following fall-off parameters has been made by Mitroy *et al.* [12]: $\rho_0 = 1.1795$, $\rho_1 = 1.302$, $\rho_2 = 1.442$, $\rho_3 = 1.52$, $\rho_{l\geqslant 4} = 1.361$, and $\rho_d = 1.361$. Cross sections obtained with this choice of polarization potential parameters have been calculated and compared with our previous results. We find that that both calculations produced practically the same results. Finally, we have performed calculations with all polarization potentials set to zero ($\alpha_d = 0.0$). This leads to a structure model that is not as accurate, for example, ionization energy is 7.5 eV, the $(3s3p)^1P^o$ excitation energy is 4.28 eV and the Mg static dipole polarizability is 74.5. We find again very close agreement with our previous calculations.

Next we turn to verifying the convergence of our calculations with respect to the quality of the discretization of the target continuum. We expect that direct ionization of magnesium by positron impact will have similar properties to electron impact ionization. This indeed has been the case for a number of other targets such as helium [23] and heavier noble gases [27]. Our previous studies of the electron impact

ionization within the CCC method indicate that convergence in TICS can be achieved relatively fast [13,14]. The unitarity of the CCC formalism ensures that the close-coupling expansion does not have to have target states with large values of angular momentum, often $l_{\max} = 3$ is sufficient and corresponding values of N_l do not have to be too large as target states with small positive energy have significantly larger cross sections. Therefore, in the case of positron scattering from atoms the convergence of the calculations with respect to N_l, λ_l, and $l_{\max}$ is a test of how well the single center close-coupling expansion models positronium formation channels.

Discretization of the target continuum for a given value of $l_{\max}$ is determined by the N_l and λ_l parameters. A number of calculations have been performed to verify the stability of the calculated cross sections with respect to these parameters. For example, we changed the value of the Laguerre function exponential fall-off parameters [see Eq. (1)] to $\lambda = 4.0$. The Mg structure model that follows has less negative energy states while positive energy states extend to higher energies compared to the model with $\lambda = 3.0$. In another model we keep $\lambda = 4.0$ and change the number of orbitals in diagonalization to $N_l = 18 - l, l = 0, \ldots, 14$. The major difference is that this will produce significantly less target states with large values of angular momentum compared to the original model. We find very good agreement between all three models at all energies, with the expected exception in the region between the Ps and IP thresholds. Of particular significance is that the results in the region of the resonance (0.17 eV) are very stable.

We have performed a detailed study of convergence of our calculations with respect to $l_{\max}$ (see Fig. 3). Calculations with $l_{\max}$ from 8 to 20 are presented. At incident energies above the IP we find that the cross section converges fast as $l_{\max}$ increases and does not significantly change for $l_{\max} \geqslant 8$. At the problematic energy range previously discussed there is no obvious convergence, even for up to $l_{\max} = 14$. However, at the low energies there is a clear pattern of convergence as the resonance peak gradually takes shape. It required an $l_{\max}$ of 20 before achieving a convergent result to within a percent or so.

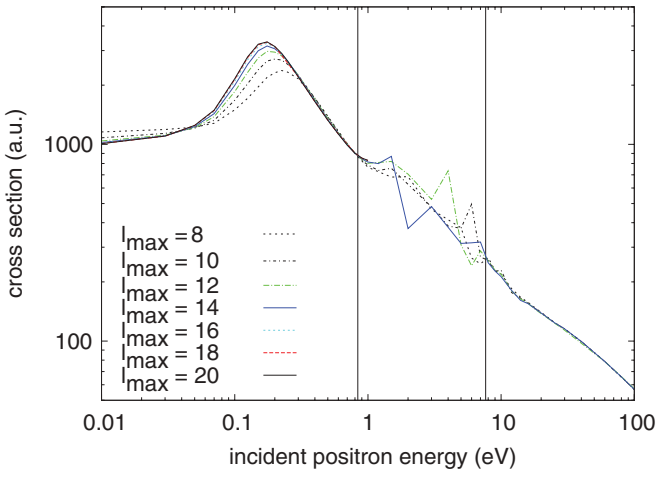

FIG. 3. (Color online) Convergence with $l_{\max}$ of positron-magnesium total cross sections calculated using the single-center CCC theory, see text. At energies above the ionization threshold (7.6 eV) the results are indistinguishable for all considered $l_{\max}$.

Such high values of $l_{\max}$ are necessary in the CCC method to model virtual positronium formation channels implicitly via the single-center close-coupling expansion.

C. Total ionization and positronium formation cross sections

In the CCC method the TICS is calculated as a sum of cross sections for all positive energy states. In the single-center method TICS represents a sum of direct ionization and positronium formation. Just like the TCS, the calculated TICS proved to be insensitive to the choice of polarization potentials and the CI expansion variations. However, at energies close to the ionization threshold it is sensitive to the details of the continuum discretization, in particular to the choice of exponential fall-off parameters in Eq. (1). The results obtained with the smaller values of the fall-off parameter are preferable as they produce more positive energy states with small energy. We find that convergence with respect to $l_{\max}$ is fast with $l_{\max} = 8$ results being barely distinguishable from $l_{\max} = 14$.

The CCC-calculated TICS should provide an accurate upper limit to both positronium formation and direct ionization cross sections. At large incident positron energies the positronium formation is negligible and the calculated TICS is the direct ionization cross section. At low energies, just above the IP threshold, the TICS corresponds to mostly Ps formation. Assuming that the Born approximation for direct ionization is not too inaccurate, we can then make a reasonable estimate of the Ps-formation cross section by subtracting the Born estimate from the CCC-calculated TICS. These cross sections are presented in Fig. 4. We see that the Born based estimate is correct at the highest energies, and is probably within 20% accuracy at all considered energies. The CCC-calculated TICS are presented at an energy range just above the direct ionization threshold where they are reasonably convergent. In the single center model the TICS should converge to a step function, being zero below the threshold and being pure Ps formation just above the threshold. The CCC-calculated estimate of the Ps-formation cross section is consistent with the experiment of Surdutovich *et al.* [3] and the calculations of Hewitt *et al.* [9].

D. Elastic and excitation cross sections

In Fig. 5 we present cross sections for elastic scattering at incident positron energies above the ionization threshold, that is, where Ps formation is adequately treated. Our CCC results are compared with present CC (no Ps formation or direct ionization), POM calculations of Campeanu *et al.* [6], and with two center five-state CCA results of Hewitt *et al.* [9].

There is good agreement between CCC and POM for elastic scattering at the lower and higher energies, with some variation at the intermediate energies. The fact that CC and CCA agree so well with each other, but not with CCC, indicates that the inclusion of the direct ionization channels can be important, even for elastic scattering.

The results for excitation of $3\,^1P$ are given in Fig. 6. The DWA results of Campeanu *et al.* [6] are substantially higher compared to the results of close-coupling calculations. We find the CCC results are generally substantially lower than the CC results. Such behavior was also identified by Hewitt *et al.* [9]

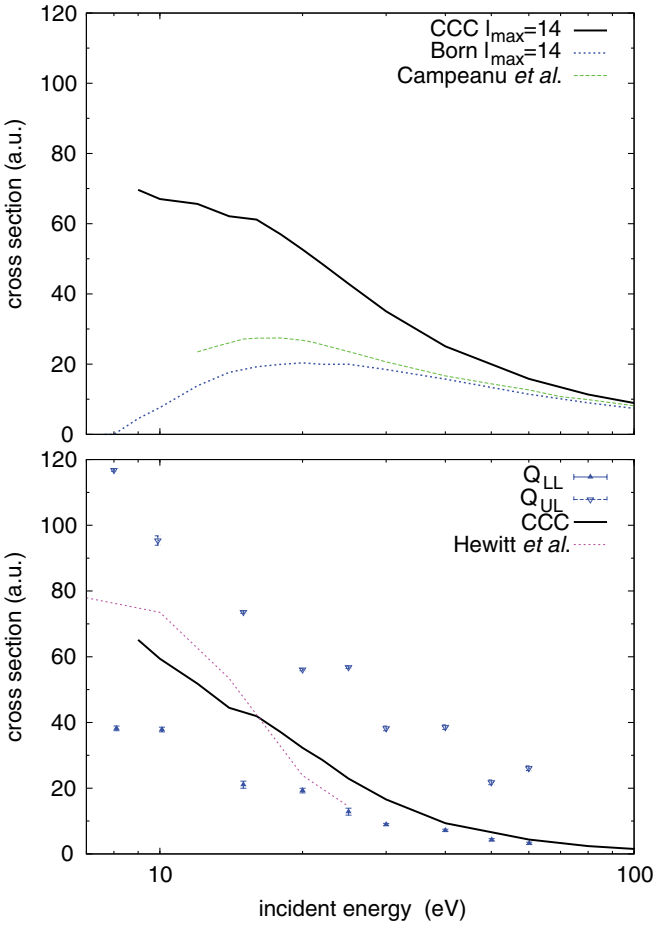

FIG. 4. (Color online) Top, positron-magnesium total ionization cross section calculated via the CCC method (Ps formation plus direct ionization), and estimates of the direct ionization via the Born approximation and the calculations of Campeanu *et al.* [6]. Bottom, the single-center CCC estimate of Ps formation derived by subtracting Born from CCC in the top panel, the calculations of Hewitt *et al.* [9], and the measurements of Surdutovich *et al.* [3], where Q_{UL} is the upper bound and Q_{UL} the lower bound of the Ps-formation cross sections.

who compared their CCA results (which included coupling to three positronium states) with the results of two-state single-center close-coupling calculations. Strong coupling to positron formation channels is responsible for the observed substantial reduction of the excitation cross sections and the increase of the elastic scattering cross section.

IV. SUMMARY

A single-center convergent close-coupling approach has been applied to study positron-magnesium scattering. Good agreement was found with the total cross section measurements of Stein *et al.* [2] for incident positron energies above the ionization potential. At energies below the positronium formation threshold, we also predict a *p*-wave shape resonance at 0.17 eV similar to that predicted by Mitroy *et al.* [12] at 0.1 eV. Detailed studies have been conducted to verify the convergence of our results. The reason for the discrepancy in the resonance position remains unclear.

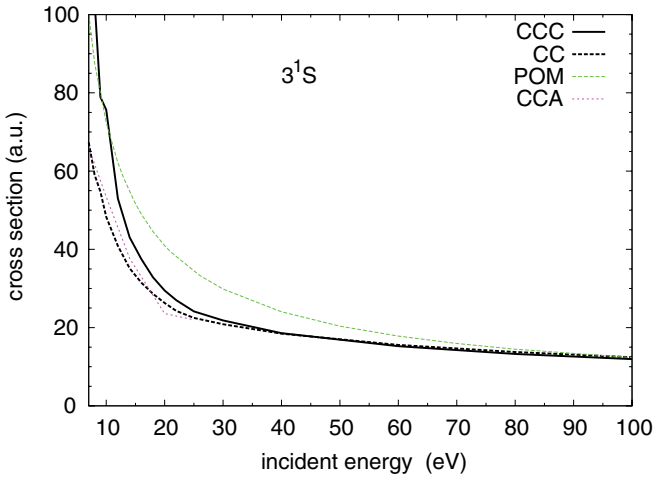

FIG. 5. (Color online) Elastic scattering cross section for positron impact on the ground state of magnesium. Present CCC and CC calculations are described in the text. Also shown are calculations due to Campeanu *et al.* [6] (POM) and Hewitt *et al.* [9] (CCA).

We have presented an estimate of the positronium formation cross section for incident positron energies above the ionization threshold, even though such channels are not explicitly included. Our results are consistent with the measurements of Surdutovich *et al.* [3], though the large experimental uncertainties do not allow for stringent verification. Cross sections for elastic scattering and excitation of $3\,^1P$ have also been presented in the energy region above the ionization threshold. The importance of coupling to ionization and positronium formation channels has been highlighted.

We hope that our results will stimulate further theoretical and experimental study of this collision system, particularly

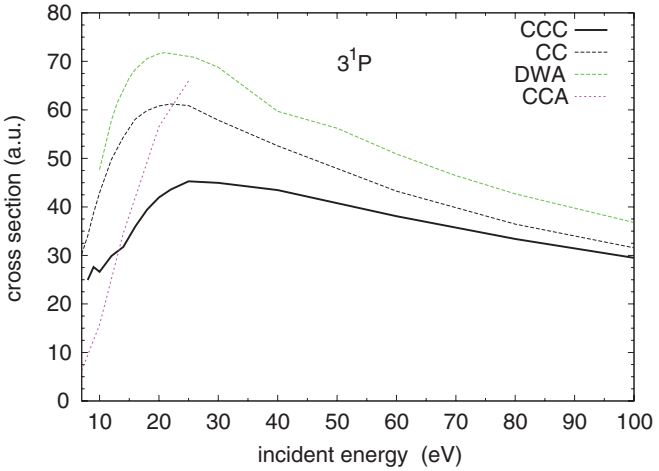

FIG. 6. (Color online) Cross section for excitation of $3\,^1P$ state by positron impact on the ground state of magnesium. Present CCC and CC calculations are described in the text. Also shown are calculations due to Campeanu *et al.* [6] (DWA) and Hewitt *et al.* [9] (CCA).

at the low energies where the elastic cross section is predicted to have an extraordinarily large maximum. We are presently extending the positron-helium two-center CCC method to the positron-magnesium case. This is a difficult task due to the fact that interactions with the core can no longer be treated analytically.

ACKNOWLEDGMENTS

This work was supported by the Australian Research Council and Curtin University. Resources of the Australian National Computational Infrastructure (NCI) Facility and its Western Australian node iVEC are gratefully acknowledged.

[1] C. M. Surko, G. F. Gribakin, and S. J. Buckman, J. Phys. B **38**, R57 (2005).
[2] T. S. Stein, M. Harte, J. Jiang, W. E. Kauppila, C. K. Kwan, H. Li, and S. Zhou, Nucl. Instrum. Methods Phys. Res. Sect. B **143**, 68 (1998).
[3] E. Surdutovich, M. Harte, W. E. Kauppila, C. K. Kwan, and T. S. Stein, Phys. Rev. A **68**, 022709 (2003).
[4] T. S. Stein, J. Jiang, W. E. Kauppila, C. K. Kwan, H. Li, A. Surdutovich, and S. Zhou, Can. J. Phys. **74**, 313 (1996).
[5] R. Szmytkowski, J. Phys. II **3**, 183 (1993).
[6] R. I. Campeanu, R. P. McEachran, L. A. Parcell, and A. D. Stauffer, Nucl. Instrum. Methods **143**, 21 (1998).
[7] M. W. J. Bromley, J. Mitroy, and G. Ryzhikh, J. Phys. B **31**, 4449 (1998).
[8] G. G. Ryzhikh, J. Mitroy, and K. Varga, J. Phys. B **31**, 3965 (1998).
[9] R. N. Hewitt, C. Noble, B. H. Bransden, and C. J. Joachain, Can. J. Phys. **74**, 559 (1996).
[10] G. F. Gribakin and W. A. King, Can. J. Phys. **74**, 449 (1996).
[11] J. Mitroy and M. W. J. Bromley, Phys. Rev. Lett. **98**, 173001 (2007).
[12] J. Mitroy, J. Y. Zhang, M. W. J. Bromley, and S. I. Young, Phys. Rev. A **78**, 012715 (2008).
[13] I. Bray and A. T. Stelbovics, Phys. Rev. A **46**, 6995 (1992).
[14] D. V. Fursa and I. Bray, Phys. Rev. A **52**, 1279 (1995).
[15] D. V. Fursa and I. Bray, J. Phys. B **30**, 5895 (1997).
[16] K. Bartschat, O. Zatsarinny, I. Bray, D. V. Fursa, and A. T. Stelbovics, J. Phys. B **37**, 2617 (2004).
[17] D. V. Fursa and I. Bray, Phys. Rev. A **63**, 032708 (2001).
[18] D. V. Fursa and I. Bray, Phys. Rev. A **59**, 282 (1999).
[19] I. Bray and A. T. Stelbovics, Phys. Rev. A **48**, 4787 (1993).
[20] P. Caradonna, A. Jones, C. Makochekanwa, D. S. Slaughter, J. P. Sullivan, S. J. Buckman, I. Bray, and D. V. Fursa, Phys. Rev. A **80**, 032710 (2009).
[21] A. C. L. Jones *et al.*, Phys. Rev. A **83**, 032701 (2011).
[22] C. Makochekanwa *et al.*, Phys. Rev. A **83**, 032721 (2011).
[23] R. Utamuratov, A. S. Kadyrov, D. V. Fursa, I. Bray, and A. T. Stelbovics, J. Phys. B **43**, 125203 (2010).
[24] C. Froese-Fischer, Can. J. Phys. **53**, 338 (1975).
[25] Y. Ralchenko, A. E. Kramida, J. Reader, and NIST ASD Team, *NIST Atomic Spectra Database (version 3.1.5)* (NIST, Washington, DC, 2008).
[26] A. Derevianko, S. G. Porsev, and J. F. Babb, At. Data Nucl. Data Tables **96**, 323 (2010), ISSN 0092-640X.
[27] V. Kara, K. Paludan, J. Moxom, P. Ashley, and G. Laricchia, J. Phys. B **30**, 3933 (1997).