Internal consistency in positron-hydrogen-scattering calculations

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(Received 3 November 2014; published 29 January 2015)

Internal consistency in a close-coupling approach to positron-hydrogen scattering is investigated with a particular focus on the potential overlap between the atomic and positronium continua. We present results for total, total ionization, and 1*s* positronium-formation cross sections for projectile energies up to 100 eV. We show that, irrespective of whether the continuum is treated by one center, or the other, or both, the same cross sections are generally obtained. This is true only if sufficiently large orbital angular momentum is taken in the close-coupling expansion. Furthermore, unitarity of the close-coupling approach ensures convergence of the physically observable cross sections even if the individual components are not convergent.

DOI: 10.1103/PhysRevA.91.012712 PACS number(s): 34.80.Uv

I. INTRODUCTION

The positron-atom-scattering problem is of interest to the scientific community from both the theoretical and practical perspectives. Theoretical complexity arises from the existence of the rearrangement channel, known as positronium formation. This is more complicated than exchange processes in electron scattering due to the requirement for (at least two) separate coordinate systems. Much of the foundational work has been carried out some time ago [1–5]. On the practical side, positron scattering is important in medical imaging and materials science, with considerable recent activity [6–10]. Comprehensive reviews of the field have been given by Surko *et al*. [11], Laricchia *et al*. [12], and Chiari and Zecca [13].

The positron-hydrogen-scattering system has two natural centers, hydrogen (H) and positronium (Ps). Both have a discrete and a continuous spectrum. For positron scattering on the ground state of H, excitation of the H continuum corresponds to combined Ps formation and three-body breakup (electron loss). On the other hand the Ps continuum corresponds solely to three-body breakup, with the discrete spectrum corresponding to explicit Ps formation. Hence any complete (discrete and continuum) treatment of both centers in a close-coupling approach may potentially double count the three-body breakup scattering processes. Here our interest is to investigate this issue within the two-center convergent close-coupling (CCC) method. We require that the two-center CCC calculations be internally consistent, i.e., yield the same physical results even when substantially different expansions on the two centers are undertaken.

The CCC method was originally developed by Bray and Stelbovics [14] for electron-hydrogen scattering, with the most recent review of applications given by Bray *et al*. [15]. When first applied to the positron-hydrogen-scattering problem it did not include Ps formation, but was able to yield the correct phase shifts at low energies [16] and resolve discrepancies between experiments for total ionization at high energies [17].

The close-coupling method has been successful in treating the positron-atom-scattering problem. It has many numerical implementations [2,3,18,19]. Following the work of Mitroy [3] and Campbell *et al*. [20], Kadyrov and Bray [21] developed a two-center CCC method which explicitly includes Ps-formation channels, and obtained good agreement with experiment without any double-counting problems. This was further supported by considering convergence in the *s*-wave model, where pseudoresonances of the type identified by Higgins and Burke [18] could only be eliminated using a near-complete treatment of both centers [22]. Furthermore, application to three-body breakup near threshold showed that the contribution from both centers becomes the same as threshold approaches [23].

II. METHOD

The details of the two-center CCC formalism for positron scattering have been given in Ref. [21]. Briefly, the one-electron target (T) Hamiltonian $H_{\rm T}$ is diagonalized for each orbital angular momentum $l \leqslant l_{\max}$ to obtain target pseudostates using

$$\left\langle \phi_f^{(\rm T)} \middle| H_{\rm T} \middle| \phi_i^{(\rm T)} \right\rangle = \epsilon_f^{(\rm T)} \delta_{\rm fi}, \tag{1}$$

where the $\phi_n^{(\rm T)}(r)$ are linear combinations of the complete Laguerre basis:

$$\xi_{n,l}^{(\lambda)}(r) = \left(\frac{\lambda (n-1)!}{(2l+1+n)!} \right)^{1/2} \times (\lambda r)^{l+1} \exp[-\lambda r/2]\, L_{n-1}^{2l+2}(-\lambda r), \tag{2}$$

where $L_{n-1}^{2l+2}(x)$ is the associated Laguerre polynomial, and n ranges from 1 to the basis size N_l. With increasing N_l the negative-energy states converge to the true discrete eigenstates, while the positive-energy states yield an increasingly dense discretization of the target continuum. Explicit inclusion of Ps (pseudo)states also requires diagonalization of the Ps Hamiltonian in a Laguerre basis:

$$\left\langle \phi_f^{(\rm Ps)} \middle| H_{\rm Ps} \middle| \phi_i^{(\rm Ps)} \right\rangle = \epsilon_f^{(\rm Ps)} \delta_{\rm fi}. \tag{3}$$

To get the scattering cross sections we solve the set of momentum-space coupled Lippmann-Schwinger equations for the transition-matrix elements:

$$T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_{\gamma}) = V_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_{\gamma}) + \sum_{\gamma''}^{N^{(\rm T)}+N^{(\rm Ps)}} \int \frac{d\boldsymbol{q}_{\gamma''}}{(2\pi)^3} \times \frac{V_{\gamma',\gamma''}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_{\gamma''}) T_{\gamma'',\gamma}(\boldsymbol{q}_{\gamma''},\boldsymbol{q}_{\gamma})}{E + i0 - \epsilon_{\gamma''} - q_{\gamma''}^2/(2M_{\gamma''})}, \tag{4}$$

where E is the total energy, $\boldsymbol{q}_\gamma$ is the momentum of the free particle γ relative to the c.m. of the bound pair in channel γ (H or Ps), ϵ_γ is the corresponding energy of the bound pair, M_γ is its reduced mass, and $V_{\gamma',\gamma}$ is the effective potential [21].

The set of integral equations (4) is solved using the partial-wave expansion in total orbital angular momentum.

III. RESULTS AND DISCUSSION

One of the strengths of the two-center CCC formalism is the ability to check the internal consistency. Both expansions approach completeness with increasing N, but are not orthogonal. The unitarity of the close-coupling formalism ensures that double counting should not occur, but the potential over-completeness manifests itself through ill-conditioned linear equations when solving Eq. (4). Thus, we cannot arbitrarily increase our basis sizes, but need to be particularly careful in demonstrating convergence.

At the very low energies where only elastic scattering is possible only the target ground state is open. All other states are closed, and correspond to virtual excitation, ionization, and Ps formation. These virtual effects can be very large and, due to the completeness of the Laguerre basis, can be treated by either center. This is a very good but a somewhat indirect test of the two-center formalism, and has been performed previously [16]. As we are interested in the interplay between the continuum of H and that of Ps, here we will concentrate on energies above the ionization threshold.

The critical aspect of the CCC approach is to demonstrate convergence at each energy of the projectile with increasing basis size parameters N_l and $l_{\max}$, for specified exponential falloff λ_l. We are free to vary N_l and λ_l for each l, for both the H target and Ps. This creates considerable flexibility, but for the purpose of a clear presentation of the convergence we take $\lambda_l^{(\mathrm{Ps})}$=1 and $\lambda_l^{(\mathrm{H})} = 2$ in all presented calculations. This yields exact Ps($1s$) and H($1s$) with $N_0^{(\mathrm{Ps})} = N_0^{(\mathrm{H})} = 1$. We will demonstrate convergence by variation of N_l and $l_{\max}$ for each center.

The bases used in this work are denoted as CCC(N_0^{H},N_0^{Ps},$l_{\max}$), where $l_{\max}$ is the maximum orbital angular momentum of the target and Ps states. For each l, the number of included pseudostates is $N_0 - l$. We consider the four bases CCC($\overline{30}$,0,9), CCC($\overline{20}$,$\overline{20}$,2), CCC($\overline{20}$,4,3), and CCC(8,$\overline{25}$,2), where each basis represents the three-body continuum in a different way, and is chosen to give a convergent final result. A bar indicates the use of pseudostates and no bar means only exact bound states are included. The first calculation has a near-complete set of H (pseudo)states, but has no Ps states. The second has an equally distributed number of pseudostates across both centers. The third has a near complete set of H (pseudo)states with just a few Ps bound eigenstates. Finally, the fourth calculation has a near-complete expansion of Ps (pseudo)states with few H bound eigenstates. The last is particularly noteworthy because this is the first time that the CCC calculations were performed in this way, and we are unaware of any other method that has attempted such calculations. All four bases were used to perform e^+-H calculations for partial waves of total orbital angular momentum ranging from zero to twenty over the full energy range. The full, summed over all partial waves, results are much the same as those presented previously [21]. Here, for the purpose of this study the zeroth partial wave is representative of the behavior within each partial wave.

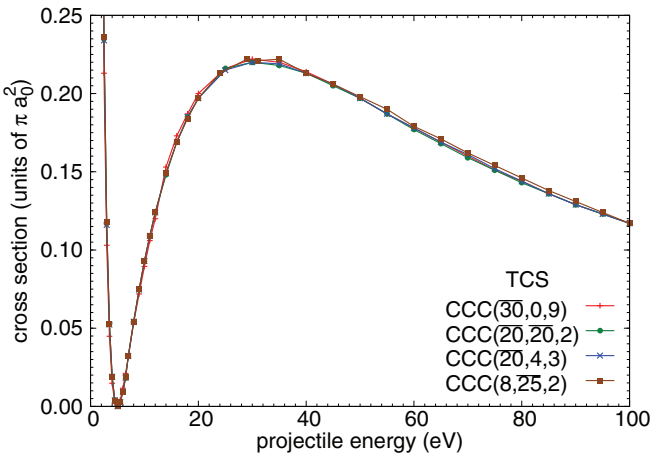

FIG. 1. (Color online) Total cross section for the zeroth partial wave of e^+-H scattering calculated with the specified CCC(N_0^{H},N_0^{Ps},$l_{\max}$) calculations (see text).

In Fig. 1 we present the four sets of calculations for total cross sections (TCS). Excellent agreement between them is a necessary starting point which says that all physical cross sections, when summed, give the same result. At the lower energies elastic scattering dominates, but virtual Ps formation is very important. Implicit inclusion via $l_{\max} = 9$ in the single center CCC($\overline{30}$,0,9) calculation, or explicit inclusion of Ps states in the other three bases, provides an equivalent treatment.

An even more interesting case is the total ionization cross section (TICS) presented in Fig. 2. This is a combination of Ps-formation and breakup cross sections. The CCC($\overline{30}$,0,9) calculation yields this cross section by simply summing the excitation cross sections for all of the positive-energy atomic

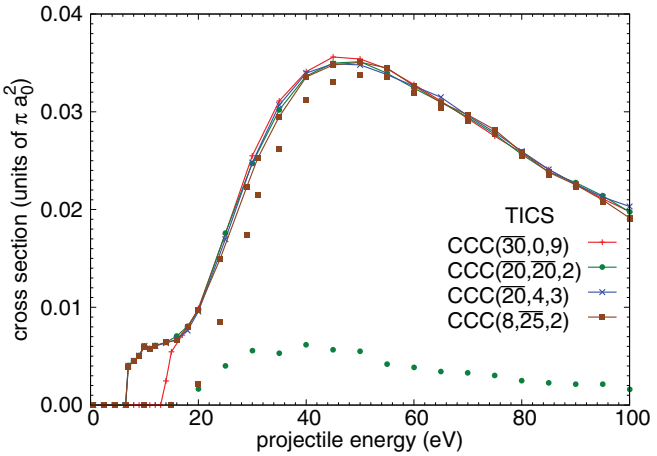

FIG. 2. (Color online) Same as Fig. 1, except for the total ionization cross section (Ps formation plus breakup cross sections). The individual unconnected points indicate the contribution from the Ps continuum.

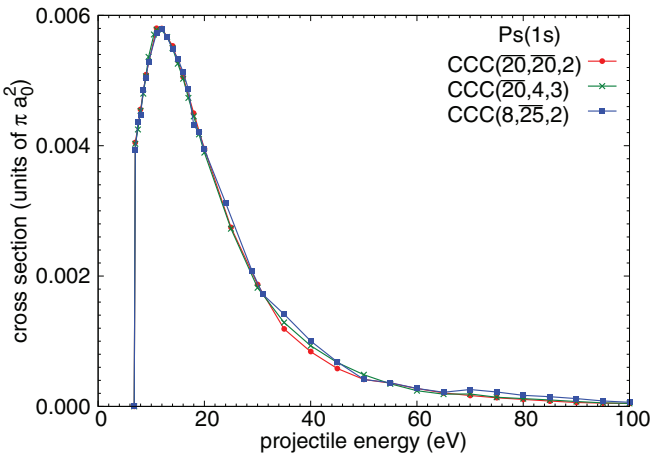

FIG. 3. (Color online) Same as Fig. 1, except for the Ps(1s) formation cross section.

states. It needs the large $l_{\max}$ and N_l near the ionization threshold as it should yield a near step function with the positive-energy cross sections yielding the total Ps formation at the step height (the breakup cross section is zero at threshold). The absence of explicit Ps formation is why this cross section starts at 13.6 eV. The other three two-center calculations start at the Ps(1s) formation threshold and quickly converge to the single center CCC result. To show how remarkable that is we also present the individual contributions from the Ps continuum, which is nonzero only in the CCC($\overline{20}$,$\overline{20}$,2) and CCC(8,$\overline{25}$,2) calculations. In the case of CCC($\overline{20}$,$\overline{20}$,2) this is relatively small, with the majority of the contribution to the TICS (not shown) coming from the cross sections for excitation of the positive-energy atomic states, with the remainder coming from the Ps bound states. However, in the CCC(8,$\overline{25}$,2) case, where there are no positive-energy atomic states, the contribution from the positive-energy Ps states is enormous, with the remainder being due to Ps formation. Clearly, there is no convergence in the individual components, yet the four calculations give an almost identical TICS at energies above the ionization threshold. It is the unitarity of the close-coupling formalism that ensures convergence in the physically observable cross sections.

To complete the task of checking the internal consistency we consider the Ps(1s) formation cross section in Fig. 3. Only the three calculations that explicitly include Ps states generate this cross section. Given that this is a relatively small cross section it is a particularly sensitive test of the two-center CCC formalism. Nevertheless, we see generally good agreement between the three calculations.

IV. CONCLUSION

Given the vastly different set of states included, such broad agreement between the diverse calculations allows us to draw some solid conclusions.

First, we note that there were no unphysical resonances found in the present study, as discussed earlier when only $l = 0$ states were included [22]. This indicates that the inclusion of a substantial $l_{\max} > 0$ has resolved this problem. Given that Ps formation is electron-positron correlation away from the atomic center it is not surprising that substantial $l_{\max}$ is required for convergence.

Second, unitarity of the CCC formalism is responsible for obtaining convergent physical cross sections, even when individual components are not convergent. In this sense this is similar to the case found in electron-sodium scattering, where the total ionization cross section converged much faster than its individual components [24]. However, in the present study there is the greater complexity in that the contribution to the three-body breakup channel can come from the atomic center, the positronium center, or both.

The internal consistency checks presented here rely on the ability to calculate the underlying matrix elements [21] to a very high precision. This is required to deal with the ill-conditioned sets of equations arising when the three-body continuum is treated by both centers. It is our goal to be able to do the same for e^+-He scattering using the two-center CCC method [25]. However, as yet we are unable to do so. This is a four-body problem where Ps is formed in the field of He^+ requiring the treatment of excitation, virtual or real, and electron exchange with the Ps electrons. While problems are evident in the lowest partial waves, when summed over all partial waves they become negligible and agreement with experiment is excellent [25]. This indicates the importance of performing the kind of internal consistency study presented here, with the results acting as benchmarks for any new approaches to the problem.

Finally, the internal consistency we have established here was for discrete channels, including Ps formation and total ionization. However, the effect of two-center expansions on differential breakup cross sections remains an ongoing challenge; see Kadyrov *et al.* [26] for some preliminary discussion. Full understanding of this aspect would be an important step toward solving the genuine three-body problem that is e^+-H scattering.

ACKNOWLEDGMENTS

We acknowledge the support of the Australian Research Council. This research was undertaken with the assistance of resources from the National Computational Infrastructure and the Pawsey Supercomputer Center in Western Australia.

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