Near-Threshold Positron-Impact Ionization of Atomic Hydrogen

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We consider the positron-impact ionization (breakup) of atomic hydrogen utilizing the full and S-wave model calculations, concentrating on the near-threshold energy region. Unlike the corresponding electron-impact case, the S-wave model does support the Wannier-like threshold law predicted by Ihra *et al.* [Phys. Rev. Lett. **78**, 4027 (1997)]. It is found that convergent S-wave model cross sections are obtained only if complete expansions are utilized on both the atomic and the positronium centers. Furthermore, we suggest that, in the model and full calculations, the separate contributions to the breakup cross section from both centers become equal at threshold.

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The breakup of three-body Coulomb systems, when the total energy is close to zero, has been attracting considerable interest of physicists for many decades. The threshold breakup phenomenon in electron-atom scattering is now considered as fairly well understood from both theoretical [1–4] and experimental points of view [5] with theory and experiment being in very good agreement. The first theory of near-threshold breakup was given by Wannier [1]. Using classical mechanics, he proposed a law for the total breakup cross section as a function of the total energy of the system, or, equivalently, the excess kinetic energy of the incident particle, known as the Wannier threshold law. Subsequently, this law was shown to hold in both semiclassical [2,4] and quantal approaches [3] and has recently been confirmed by accurate numerical calculations of electron-hydrogen scattering [6].

However, the situation is not so clear for positron-atom scattering. This system displays a genuine three-body nature, where all of the particles are distinguishable and rearrangement collisions are possible due to positronium (Ps) formation. It is a two-center collision system, whereas electron-atom scattering is a single-center one. Therefore, the positron-atom system is a more challenging test of theory and arguably more important as a prototype of the more complex multicenter collision systems.

Klar [7] extended the Wannier theory to the positron-hydrogen system. Klar's classical results were first questioned by Temkin [8] and Geltman [9], but later reconfirmed by Rost and Heller [10] in the semiclassical approximation. However, following measurements by Ashley, Moxom, and Laricchia [11] of the positron-He ionization near the threshold, the validity of the theory was questioned once more. This controversy was resolved by Ihra *et al.* [12], who refined Klar's results to the next order employing the hidden crossing theory.

The aforementioned classical and semiclassical approaches to the near-threshold breakup have given important insights into the phenomenon. However, they assume collinear alignment of the particles, and the interaction is limited to the so-called Coulomb zone, where the Coulomb potential is larger than the combined kinetic energy of the escaping electron and positron. So far, no detailed fully quantum-mechanical investigations of the problem have been reported, and it is our purpose to address this issue.

Utilizing the convergent close-coupling (CCC) method [13], we report the first fully quantal numerical calculations of positron-hydrogen scattering near the breakup threshold. The positron-impact CCC approach has already been applied to the S-wave model [14] and the full problem [15] in a wide energy range below and above the breakup threshold. The method utilizes two complete Laguerre bases for expansion of the total three-body scattering wave function. The Hamiltonians for H and Ps are diagonalized separately using two independent bases resulting in negative- and positive-energy states for the two centers. With increasing basis sizes, the negative-energy states converge to the true discrete eigenstates, while the positive-energy pseudostates provide a discretization of the H and Ps continua. Convergence in observables is obtained by increasing the basis sizes. It has been demonstrated that the two-center pseudostate close-coupling approach to the problem does lead to practical convergence [14]. This was possible only when sufficiently large pseudostate expansions were used on both the H and the Ps centers as described above. However, in these papers no particular attention was paid to the ionization threshold region.

It is noteworthy that no overcompleteness problems associated with nonorthogonal two-center expansions were found, even in the three-body fragmentation channel. This is related to the fact that cross sections are defined at infinite separation of the particles of interest, where there is no overlap of the two bases owing to their square-integrable nature. However, two complete expansions do yield highly ill-conditioned numerical equations requiring

immense computational resources, which is particularly problematic whenever the cross sections are small, as in the case of the breakup cross sections in the near-threshold region of interest here.

The breakup cross section is obtained from CCC calculations by simply summing the individual cross sections for excitation of the positive-energy states. The contributions from the positive-energy H and Ps states are entirely separate, though being a unitary theory the sum over cross sections for all states must satisfy the optical theorem.

We begin by presenting in Fig. 1 the CCC results from Fig. 8 of Ref. [15] but with a log scale on the energy axis to emphasize the lower energies. The curve denoted by CCC(H + Ps) is the CCC estimate of the total breakup cross section, with the contributions from positive-energy H and Ps states summed together, and yields generally good agreement with the experiment of Jones *et al.* [16]. The curve denoted by CCC(H) shows just the contribution of the direct ionization part coming only from the atomic positive-energy states, as reported earlier. However, here we also give the same curve but multiplied by two and denoted by CCC(H + H). The reason why the latter is given is the remarkable fact that, below about 20 eV above threshold, the CCC(H + Ps) and CCC(H + H) curves are much the same, indicating that the Ps and H contributions converge to each other as the threshold is approached, something that we missed in the description of these results earlier [15].

To study this in more detail, and to investigate the nature of the threshold law, we consider the S-wave model that retains only H and Ps s states in the $L = 0$ partial wave. This is analogous to the S-wave model of e-H scattering, known as the Temkin-Poet model [17,18]. In both cases, only states with zero orbital angular momentum are retained. However, whereas the Temkin-Poet model may be described as a spherically averaged model of e-H scattering, this is not our usage for positron scattering due to the explicit introduction of Ps states. Here we are interested in extracting the physics contained in the full calculations from as minimal a model calculation as possible.

The S-wave models play a very important role in the testing of general computational approaches. The CCC method for electron impact was first applied and tested on such a model [19], as have many others; see Refs. [20–25], for example. The model is able to test the convergence of the approach with increasing basis sizes but, for electron scattering, is known not to yield the correct Wannier threshold law.

The issue of convergence is more complicated in the case of positron scattering than electron scattering. In the latter, there are two parameters: λ, the Laguerre basis exponential falloff, and N, the basis size. For positron scattering, we have to define these for both the H and the Ps states. For brevity of presentation, we set $\lambda_H = \lambda_{Ps} = 2$ and $N_H = N_{Ps} = N$. It may be that at some energies or for some transitions a more optimal combination can be found, but this suffices to obtain convergence within the S-wave model across a broad energy range.

In Fig. 2, we present the results of the CCC calculations that have basis sizes starting at $N = 35$ above 2 eV and increasing up to $N = 45$ at lower energies. The smooth results presented are an indication of convergence.

Just as we saw for the full problem, the contributions from the positive-energy Ps and H states become equal as the threshold is approached. Additionally, the Wannier-like threshold law derived by Ihra *et al.* [12] is in good agreement with the CCC results below 1 eV excess energy. This law was derived for the $L = 0$ partial wave, and Rost and

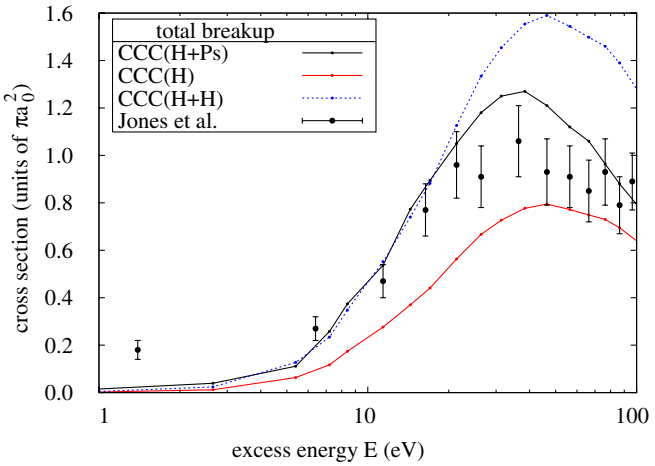

FIG. 1 (color online). Total $e^+ - H$ breakup cross section as a function of excess energy calculated using the two-center CCC method and reported by Kadyrov and Bray [15]. The argument to the CCC label indicates which center's positive-energy states were used; see text. The experiment is due to Jones *et al.* [16].

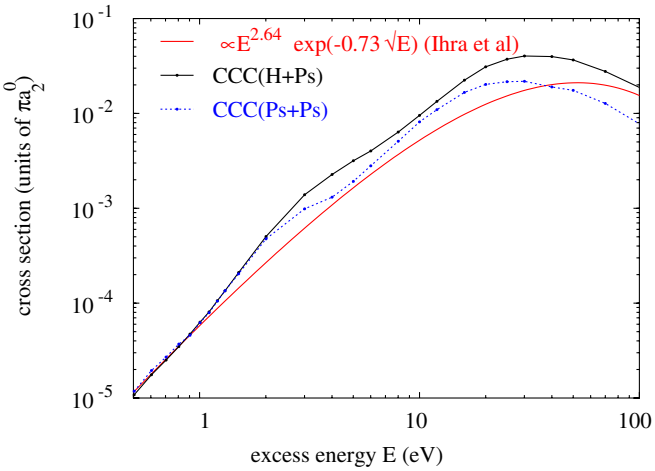

FIG. 2 (color online). Total $e^+ - H$ S-wave model breakup cross section as a function of excess energy calculated using the two-center CCC method. As in Fig. 1, the argument to the CCC label indicates which center's positive-energy states were used. The Wannier-like threshold law is due to Ihra *et al.* [12].

Heller [10] argued that the same energy dependence holds in all partial waves.

We are not able to provide accurate results at arbitrarily low energies above threshold. Increasing basis sizes even further leads to highly ill-conditioned systems that are as yet beyond our means to solve. For the full problem, we have to use smaller basis sizes due to $l > 0$ states being also included, and this does not allow the same accuracy access as close to threshold as in the S-wave model. We may try to diminish the ill-conditioning by dropping the positive-energy states on one or the other center. This makes the system of equations easier to solve but results in cross sections that show unphysical resonances of the type demonstrated earlier [14]. Thus, stable and smooth results are obtained only when complete (untruncated) bases are used on both centers.

Hence, we have two unexpected results to explain: (i) Why does the S-wave model for positron scattering yield a Wannier-like threshold law for breakup while the electron-scattering one does not? (ii) Why do the contributions to breakup from the H and Ps centers generally become equal at threshold?

We begin with the first question. We know that at threshold we expect the three-particle separation to be predominantly collinear. In electron-impact ionization calculations, this occurs by ensuring accurate electron-electron correlation at relatively large separations. This can be done only in full calculations utilizing states with nonzero angular momenta. A similar situation occurs in positron scattering. Without explicit allowance for Ps formation, electron-positron correlation would typically require states with large angular momenta; see, for example, Ref. [26] for positron-helium scattering below the Ps-formation threshold. However, if Ps states are explicitly included, even if only s states, then the positron-electron correlations are substantially accounted for. This explanation is readily tested. For example, adding $l = 1$ (or higher) states to our S-wave model calculation has no qualitative, and only a small quantitative, effect on the $L = 0$ results presented. On the other hand, for electron scattering in the Temkin-Poet model, adding $l = 1$ states has a substantial quantitative and qualitative effect on the ionization cross section. Hence, with Ref. [10], the positron-impact S-wave model, which explicitly includes Ps s states, displays the physical behavior of the full calculations near the breakup threshold. Furthermore, calculations that include Ps states explicitly require smaller l states for convergence.

Now we turn to the second question. By considering high incident positron energies, we know that the direct ionization process is going to dominate the total breakup cross section, with Ps formation diminishing rapidly with increasing energy. Here breakup is dominated by the positron exiting with most of the excess energy, leaving a slow electron, and there is little probability of forming a Ps state of any energy. However, as the excess energy diminishes towards zero, the breakup process is dominated by alignment where the electron is almost in the middle between the proton and the positron, leading to much the same interactions with both. Accordingly, in this circumstance there is no preference as to whether the electron is associated with a positive-energy atomic or Ps state. Hence, the two contributions to breakup merge in the near-threshold region.

In summary, the positron-atom collision system goes beyond the single-center electron-atom system and provides a prototype for multicenter collision systems. Consequently, it is important to come up with practical general approaches to its solution. We suggest that the usage of untruncated Laguerre-based atomic and Ps states in the expansion of the total wave function is one such approach. Even within the stated S-wave model, this yields the physical behavior for the three-body breakup in the near-threshold region, unlike the corresponding electron-scattering counterpart. The contributions to the breakup from the two centers become equal at the threshold in the model and full calculations, and perhaps this can be used as a measure of the accuracy of any similar two-center-expansion calculation.

While we have already addressed the issue of double-counting that might be expected to follow from the usage of two complete, but not mutually orthogonal, expansions, we do not know how this will affect the extraction of the ionization amplitudes. As a point of speculation, following our experience with step functions in electron scattering [27], it may be that a novel step function behavior will naturally arise that ensures that whenever positive-energy states based on one center contribute to an ionization amplitude, positive-energy states from the other center do not. Addressing these formalities will be a keen point of interest for us in the near future.

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