Estimating positronium formation for plasma applications

T. C. Naginey
Physics Department, Old Dominion University, Norfolk, Virginia 23323, USA

B. B. Pollock
Lawrence Livermore National Laboratory, California 94551, USA

Eric W. Stacy
Physics Department, Old Dominion University, Norfolk, Virginia 23323, USA

H. R. J. Walters
Department of Applied Mathematics and Theoretical Physics, The Queen's University, Belfast BT7 1NN, United Kingdom

Colm T. Whelan
Physics Department, Old Dominion University, Norfolk, Virginia 23323, USA,
and Lawrence Livermore National Laboratory, California, USA
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The basic physics of e^+,e^- creation and annihilation is overviewed. It is shown that for atomic hydrogen targets electron capture by a free positron to form positronium is vastly more probable than in-flight annihilation. Cross sections are presented using the classical trajectory Monte Carlo (CTMC) approach for the charge-exchange process:

$$e^+ + A^{q+} \rightarrow Ps + A^{(q+1)+},$$

where A^{q+} is some target ion of charge q. Charge-exchange cross sections for hydrogenic ion targets are presented. It is found that while the CTMC gives adequate results for positronium formation for e^+-hydrogen and e^+-cesium collisions, its high-energy behavior for hydrogenic ions is not in agreement with quantum mechanical predictions. Since we are interested in situations where many multicharged ions will be present we have looked for an alternative approach. Scaling rules are proposed and used to estimate the charge-exchange cross sections for both neutral atoms and multicharged ions.

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I. PAIR PRODUCTION AND ANNIHILATION

In a plasma with a large number of high-energy photons one would expect significant pair production. It is well known—see, for example, Ref. [1]—that for a photon collision with a nucleus that the pair-production cross section will be a slowly increasing function of photon energy, while the competing Compton cross section will be a rapidly decreasing function with the former dominating at high energies. The mechanism which is thought most likely to be responsible for pair production in the plasmas which are of current experimental interest was proposed by Bethe and Heitler [2]. In the first step of this process, high-energy electrons scatter off ions and produce bremsstrahlung radiation; the high-energy bremsstrahlung photons then interact with the ions and electrons in the plasma to produce electron-positron pairs. The Feynman diagram for this process is shown in Fig. 1. For an electron-positron pair to be created by a high-energy photon, its energy must be at least 1.022 MeV, since for an electron (positron) at rest $E = mc^2 = 511$ keV. Also, we will need a third particle in order to conserve momentum; working in the rest frame of the e^+,e^- pair they are moving back to back with equal energies, so we need something to carry away the initial photon momentum. This would be easiest for an ion because of its very large mass. For a photon collision with a free electron,

$$h\nu + e^- \rightarrow 2e^- + e^+, \tag{1}$$

the threshold energy will be $4mc^2$, rather than $2mc^2$, if we are to conserve both energy and momentum (see the discussion in the Appendix below).

The two step Bethe-Heitler mechanism is not the only potential source of electron-positron pairs. It has long been realized [3,4] that in Coulombic interactions at sufficiently high energies and field strengths pair production can occur. This process has been studied in relativistic heavy-ion collisions [5,6], and it can occur in highly energetic collisions between electrons and nuclei [7,8]. It is even possible to induce pair production by multi photon-photon interactions (γ-γ') [9,10]. Recently, Chen and her collaborators [11,12] succeeded in generating a dense beam of positrons by firing ultraintense, short laser pulses at a thin gold target. These authors attributed the pair production they observed to be primarily due to the Bethe-Heitler mechanism. Very recently, positrons have been observed in experiments by firing wakefield accelerated electrons into solid targets [13]. In this paper we are not concerned with the very important questions as to the mechanisms of positron creation but rather with a method to reliably estimate the behavior of the positrons once

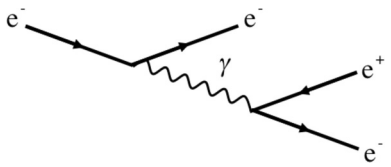

FIG. 1. Space-time diagram for the Bethe-Heitler process.

in a gas or plasma and in particular with the possibility of positronium formation and subsequent annihilation.

Given that high-density beams of positrons can now be generated, one could envisage probing a gas or plasma by firing the beam into the plasma and observing the 511-keV annihilation line and its broadening. The positrons, once created, will not immediately annihilate with the electrons in the plasma. The Dirac formula for the annihilation cross section [2,14], σ_a, is such that

$$\sigma_a \propto \frac{1}{v}, \tag{2}$$

where v is the relative speed of the positron with respect to the electron. Dirac [14] has shown that the dominant type of annihilation occurs when the positron-electron pair has zero relative total angular momentum. In this case if one photon is linearly polarized in one plane, the other photon is then linearly polarized in the perpendicular plane. Thus a coincidence measurement seeing two photons of 511 keV, at approximately 180° apart, polarized perpendicular to each other would be a clear signal of pair production [15]. However, for positrons passing through a gas at all but the lowest temperatures annihilation may not occur, rather some positrons can capture an electron to form the positronium atom, Ps.

In Fig. 2, we show a comparison between the cross sections' positron-free electron annihilation calculated in both the Heitler plane wave and Coulomb wave approximations [2] and the very accurate quantum calculations for charge-exchange formation in a collision between a positron and a hydrogen

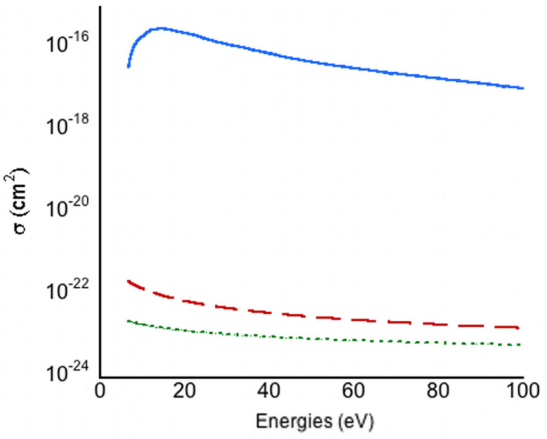

FIG. 2. (Color online) Comparison of cross sections for positron-free electron annihilation in both the Heitler plane wave (dotted line) and the Coulomb wave (dashed line) approximations [2], compared with the cross section for positronium formation in e^+,H collisions [17].

atom in its ground state [16,17],

$$e^+ + \mathrm{H}(1s) \rightarrow \mathrm{Ps} + \mathrm{H}^+. \tag{3}$$

We remark that both the positron-free electron annihilation and positronium formation cross sections are calculated in the center-of-mass frame of the projectile and target, e^+,e^- in one case and e^+,H in the other, but calculating both in the laboratory frame would in no way affect the enormous difference in the cross sections. At very low impact energies radiative recombination will further contribute to positronium formation; however, at all but the lowest energies charge exchange with the atoms in the plasma would be the dominant mechanism [18]. We thus expect that for a neutral gas the positrons will be more likely to escape or form positronium.

II. POSITRONIUM

Positronium is an "exotic atom" made up of a positron and an electron; for a review of its properties see Ref. [19]. The orbit of the two particles and the set of energy levels are similar to those of the hydrogen atom (electron and proton). The spectroscopic differences between positronium and hydrogen are due not only to the particle-antiparticle nature of Ps and the reduced mass but also to the magnitudes of the positron magnetic moment as compared to the proton magnetic moment. The magnetic moment of the positron (electron) is approximately 657 times the magnetic moment of the proton, eliminating the clear distinction between fine structure and hyperfine structure. The general selection rule for annihilation of Ps from a state of orbital angular momentum L and total spin S [19] is

$$(-1)^{L+S} = (-1)^N, \tag{4}$$

where N is the number of photons. Thus a spin singlet S state will decay to an even number of photons, while the spin triplet S state must decay to an odd number. However, the measured branching ratios show that the two-photon (singlet) and three-photon (triplet) decays are vastly more probable than any other decay mechanisms. The lowest-lying states are $1S$ spin singlet and spin triplet: the spin-singlet state $^1S_0$ (termed parapositronium) has a lifetime of 125 ps and will decay into two photons; the spin triplet state $^3S_1$ (termed orthopositronium) will produce three photons and has a lifetime of 145 ns. The first excited state $2S$ is metastable with a lifetime of 1.1 μs. It will cascade down to the "ground state" which will then annihilate as described above.

Since the reduced mass of Ps is half that of H, the atomic-energy-level transition wavelengths are twice the corresponding H series; for example, Ps Lyman α has a wavelength of 2431 Å and Ps Balmer α has a wavelength of 1.313 μm. The "fine structure" wavelengths are well known but, because of the difference between the magnetic moments of the positron and proton, are not so simply deduced from the hydrogen values (see Ref. [19]). Note that the annihilation rate depends upon the overlap of the electron-positron wave functions and thus decreases for the more highly excited states of the atom. For $2S$-ortho-Ps the lifetime is 1 μs and for non-S states it is even longer. Wheeler [15] has shown that the annihilation lifetimes of excited S-states scale like n^3. Because of the reduced mass the radiative lifetimes are almost exactly

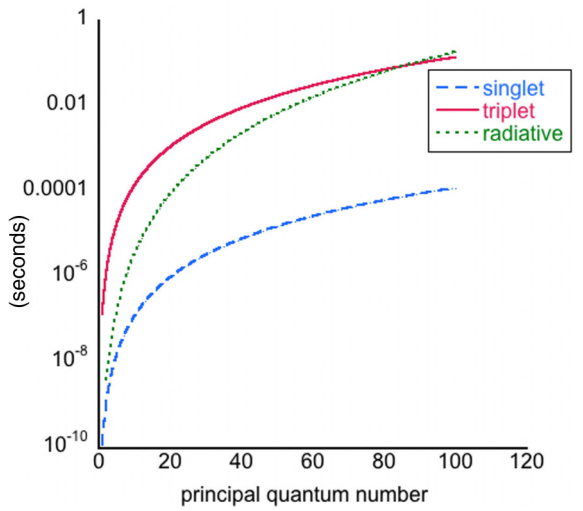

FIG. 3. (Color online) Annihilation lifetimes of the spin singlet and triplet states and radiative lifetimes for different Ps principal quantum numbers.

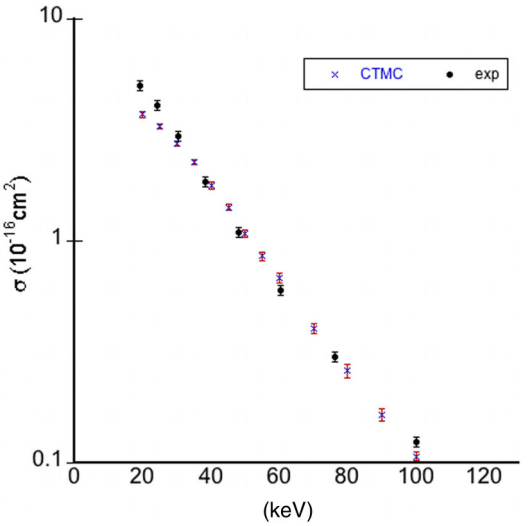

FIG. 4. (Color online) Our CTMC total charge-exchange cross section calculations (x's with statistical error shown) for proton on hydrogen compared with the experimental data of Ref. [23] (solid circles). Neither theory nor experiment gives information about which n level the electron is captured into.

twice those of hydrogen which are well known. In Ref. [20] there is a universal formula for hydrogenic systems which we have used to calculate the positronium radiative lifetimes. The radiative and annihilation lifetimes can be very different. In Fig. 3 we compare the radiative and annihilation lifetimes for the different principal quantum numbers.

Highly accurate, fully quantal coupled pseudostate calculations have been performed for positronium formation in collisions between positrons and hydrogen as well as ground state alkali-metal targets [16,17,21]. Performing equivalent close-coupling calculations would be entirely impractical for the large number of different targets and ion states that are characteristic of systems of current interest. Our ambition here is to find a relatively simple way of estimating the cross section which we can eventually incorporate into plasma simulations. Ideal for our purposes would be a method that can be evaluated rapidly and that returns cross sections of at least moderate accuracy. As a first attempt we have chosen the well-known classical trajectory Monte Carlo (CTMC) method. We found that it gave reasonable results for positron-hydrogen and positron-cesium collisions, but as is explained below we fear that it is probably less reliable for multicharged ions. As an alternative we propose a simple scaling rule which when combined with accurate hydrogen data gives us a simple and modestly reliable way of finding the cross sections needed.

III. OUTLINE OF THE CTMC METHOD FOR PROJECTILE-HYDROGEN COLLISIONS

The CTMC approach is in essence a computer experiment. In this method exact classical dynamics are performed on trajectories whose initial conditions are chosen from a classical ensemble. The initial energy of the target atom is fixed from known quantum mechanical energies, e.g., $E_0 = -0.5$ atomic units (a.u.) for hydrogen. It is assumed that the initial coordinates and momenta are uniformly distributed in phase space on this energy shell; this condition effectively defines the classical microcanonical distribution. Remarkably, Fock [22] showed that the quantum mechanical probability distribution in momentum space for the nth level of the hydrogen atom is given, in atomic units, by

$$\rho_n(\mathbf{p}) = \sum_{ml} \psi *_{nlm}(\mathbf{p})\psi_{nlm}(\mathbf{p})$$

and is equal to

$$= \frac{8p_n^5}{\pi^2}\frac{1}{\left(p_n^2 + p^2\right)^4}, \tag{5}$$

where $p_n^2 = 2|E_n|$, and the identical distribution follows from the classical microcanonical distribution [24].

In Fig. 4 we show the total cross section calculated using the CTMC method for the process

$$\mathrm{H}^+ + \mathrm{H}(n = 1) \rightarrow \mathrm{H} + \mathrm{H}^+, \tag{6}$$

where the final principal number of the captured electron is not specified. These results are in agreement both with experiment and other CTMC calculations [25] and encourage us in the use of the method for the positron charge-exchange process:

$$e^+ + \mathrm{H}(n = 1) \rightarrow \mathrm{Ps} + \mathrm{H}^+. \tag{7}$$

The classical nature of the CTMC approach means that there is capture into all states of the positronium. The accuracy we can expect from the CTMC method is open to dispute; certainly at low-impact energies near threshold one would expect that the electron will tunnel through the potential barrier it encounters. This is a quantum mechanical process, and therefore entirely absent from the CTMC. At the other extreme of very high energies all classical calculations have the wrong asymptotic behavior [5].

Error estimate

There are three main sources of error inherent in the CTMC method that are associated with the calculation of cross sections for charge transfer: (i) the error due to beginning and ending each simulated scattering event (or "run") with the incident particle and the target at a finite distance from each other, (ii) the error due to the nonzero step-length in the numerical Runge-Kutta integration of the equations of motion, and (iii) the statistical error, which decreases with the total number of runs evaluated. Errors (i) and (ii) can be controlled explicitly by two parameters in the input of the CTMC program, called γ and ϵ in Refs. [26,27], while error (iii) can only be reduced by increasing the number of runs that our program cycles through for each incident energy. As in Refs. [26,27], our CTMC program calculates the error associated with the choice of γ and ϵ after each run, and these data are included in the output. The associated errors are calculated by evaluation of the difference between the initial and final total energies of the system and so are a measure of how badly each run violates conservation of energy as a result of either γ or ϵ. Once these errors are less than the statistical error, we work with these choices of γ and ϵ.

The statistical error associated with the cross sections is deduced from a binomial distribution and is calculated by the CTMC program [26,27]. Let us denote a particular event (such as charge transfer) by q and the number of occurrences of that event by n_q, then if n is the total number of runs the statistical error associated with the cross section for q is given by

$$\sigma_q \left(\frac{n - n_q}{n_q n} \right)^{\frac{1}{2}}, \tag{8}$$

where σ_q is an estimate of the cross section for q, and is defined by

$$\sigma_q = \frac{n_q}{n} \pi b_{\max}^2, \tag{9}$$

where $b_{\max}$ is the impact parameter beyond which event q no longer occurs. The maximum statistical error is then

$$\frac{1}{2\sqrt{n}} \pi b_{\max}^2 \tag{10}$$

and occurs when $n_q = \frac{1}{2}n$. Given the statistical nature of the CTMC it is appropriate to include error bars corresponding to the statistical errors when presenting calculations.

IV. HYDROGENIC TARGETS

Because of its classical nature the CTMC does not readily yield information as to which quantum state of the positronium the electron is captured into. To estimate this we follow the method outlined in Ref. [28]. We calculate the binding energy $U = -E$ and assign a "classical principal quantum number," n_c, according to

$$U = \frac{1}{2n_c^2} \text{ a.u.} \tag{11}$$

The classical values are then "quantized" to a specific n level if

$$\left[(n-1)\left(n-\tfrac{1}{2}\right)n\right]^{\frac{1}{3}} \leqslant n_c \leqslant \left[(n+1)\left(n+\tfrac{1}{2}\right)n\right]^{\frac{1}{3}}. \tag{12}$$

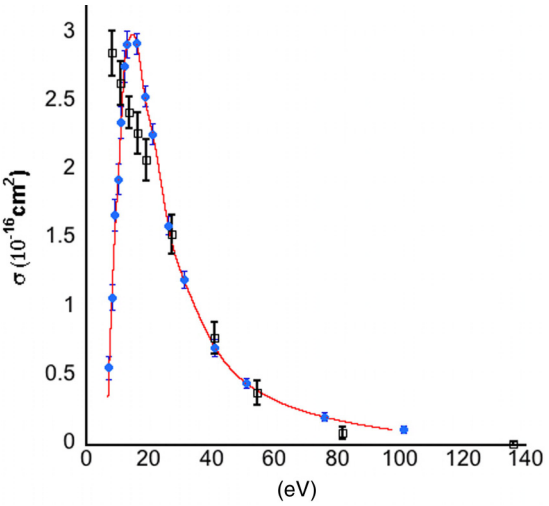

FIG. 5. (Color online) Our CTMC total charge-exchange cross section calculations, for positron on ground-state hydrogen (open squares, showing statistical error), compared with the experimental data of Ref. [29] (filled circles) and the coupled pseudostate calculation of Refs. [16,17] (dashed line).

In Fig. 5 we show our CTMC calculations compared with the experiment of Zhou *et al.* [29]. As we approach threshold the CTMC begins to fail, as it does not recognize the sharp quantum threshold and has no way of including tunneling effects. Below 10 eV our errors became unacceptably large and we do not present results below this energy. Almost all the cross section is found to come from capture to the ground state, $n = 1$.

Scaling rules

For capture from hydrogen in the nth state, the CTMC satisfies a simple scaling rule [26]:

$$\sigma_n(E) = n^4 \sigma_1 \left(\frac{E}{n^2} \right). \tag{13}$$

We thus relate the capture cross section for a positron with an impact energy E acting on a hydrogen atom with principal quantum number n to the cross section for a positron with an energy $\frac{E}{n^2}$ acting on a ground-state hydrogen atom, which is exactly n^4 times the equivalent $n = 1$ cross section.

In Fig. 6 we show our CTMC calculations for the first few hydrogenic ions. As might be expected, the cross section falls precipitously as we increase the nuclear charge Z. Jiao *et al.* [30] have performed perturbative calculations on the hydrogenic sequence with $1 \leqslant Z \leqslant 9$ and found over a quite wide range that

$$\sigma_Z(E) = \frac{1}{Z^7} \sigma_H(Z^2 E). \tag{14}$$

The same scaling formula was found by Fojón *et al.* [31]. Our CTMC calculations fall off like Z^{-4}. Unfortunately, experience has shown that the CTMC gives a poor result for protons on He^+ and Li^{2+} [5]; consequently, we are inclined to the view that most likely the CTMC will not give a good estimate for high energies and high Z. This discourages us from using the CTMC for positronium formation in positron

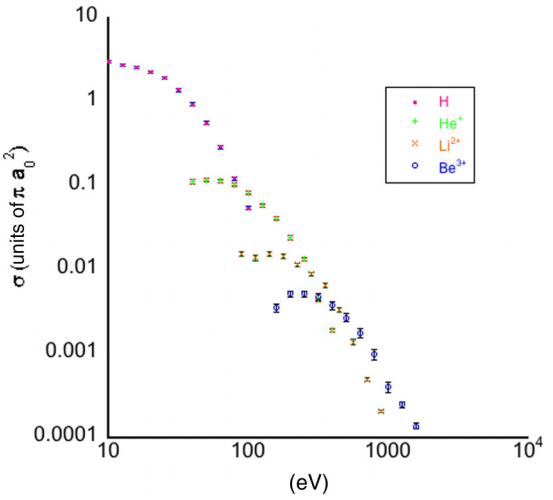

FIG. 6. (Color online) Our CTMC total charge-exchange cross section calculations, with statistical errors, for positron on ground-state hydrogenic ions: filled circles, neutral hydrogen; +, He^+; ×, Li^{2+}; open circles, Be^{3+}.

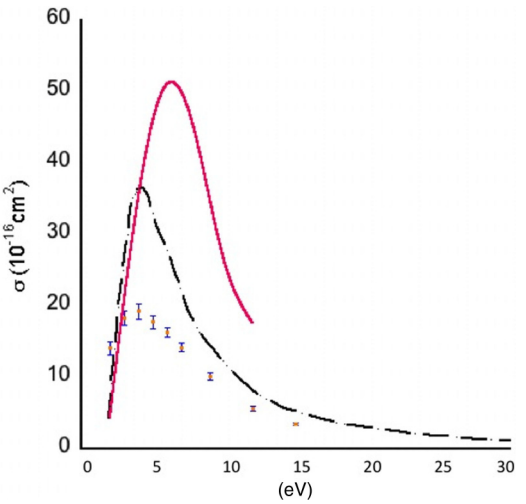

FIG. 7. (Color online) The charge-exchange cross section for e^+ on neutral cesium calculated using Eq. (17) (dashed line) and CTMC (solid squares with error bars) compared with the coupled pseudostate calculations of Kernoghan *et al.* [21] (solid line).

collisions from other than neutrals and we must look elsewhere for a source of modestly accurate cross sections which one could include in plasma simulation codes. Our idea is to look for scaling rules which will allow us to use the cross sections for hydrogen, where there is excellent agreement between theory and experiment, to estimate the cross section for a range of atoms and ions.

We will assume that Eq. (14) is valid for all hydrogenic ions and from it we can relate the cross section for positronium formation arising from a positron with an impact energy E acting on a hydrogenic ion with nuclear charge Z, giving rise to a cross section of Z^{-7} times the equivalent neutral cross section for an impact energy of Z^2E. Combining Eqs. (13) and (14), we have, for a hydrogenic ion of nuclear charge Z in the nth level,

$$\sigma_A(E) = \frac{n^4}{Z^7}\sigma_H\left(\frac{Z^2}{n^2}E\right). \tag{15}$$

We can write Eq. (15) in an equivalent form. For an electron in the nth level of a hydrogenic ion, its binding energy is (in atomic units)

$$E_{\text{binding}} = -\frac{1}{2}\frac{Z^2}{n^2}.$$

Let us introduce the dimensionless scaling parameter

$$\epsilon_A = \frac{I_H}{E_{\text{binding}}} = \frac{n^2}{Z^2}, \tag{16}$$

where I_H is the binding energy of an electron in the ground state of the hydrogen atom, with a numerical value of -0.5 a.u. (13.5984 eV); then we can rewrite Eq. (15) as

$$\sigma_A(E) = \frac{\epsilon_A^2}{s(Z)^3}\sigma_H\left(\frac{E}{\epsilon_A}\right). \tag{17}$$

The advantage of the form (17) is that the dimensionless scaling factor ϵ_A depends on the binding energy of the target atom: there is a great deal of physics of the atom implicitly contained in that number. The function s in Eq. (17) is defined to be

$$s(Z) = \begin{cases} 1, & \text{if neutral atom,} \\ Z, & \text{if ion of charge } Z. \end{cases}$$

V. RESULTS

A. Cesium

In this section we present results using both our CTMC and scaling method for a number of systems. There is considerable current interest in the possibility of generating beams of long-lived positronium atoms [32,33] by means of positron impact on cesium. In Fig. 7 we show our scaled results compared with both the CTMC and the coupled pseudostate calculation of Ref. [21]. Agreement between the three approaches is adequate. In the CTMC calculation we treated the Cs as a hydrogenlike atom with an experimentally determined binding energy of 3.8939 eV and a nuclear charge of 2.2 as deduced from the Slater rules [34]. We used our CTMC code to determine the contribution that capture into the n_{Ps} makes to the total capture cross section.

For proton-hydrogen and positron-hydrogen collisions, our analysis shows that capture is predominantly into the $n = 1$ state. However, for a ground-state cesium target we found at an impact energy of 6 eV that 60% of the cross section came from capture into the $n = 2$ state, while nearly 13% came from capture into n states with $n \geqslant 4$. Kernoghan *et al.* [21] estimated that 20% of the cross section came from $n \geqslant 4$. As can be seen from Fig. 3, the triplet positronium has an annihilation lifetime of the order of 10^{-6} s for $n = 4$ and greater than 10^{-4} s for $n \geqslant 10$. Cassidy *et al.* [33] have successfully demonstrated that Ps atoms in the $2\,^3P$ state can be successfully pumped into rydberg states with $10 \leqslant n \leqslant 25$, thus dramatically increasing their lifetime. Our analysis suggests that this process could be facilitated by creating the positronium by firing positrons through a cesium vapor.

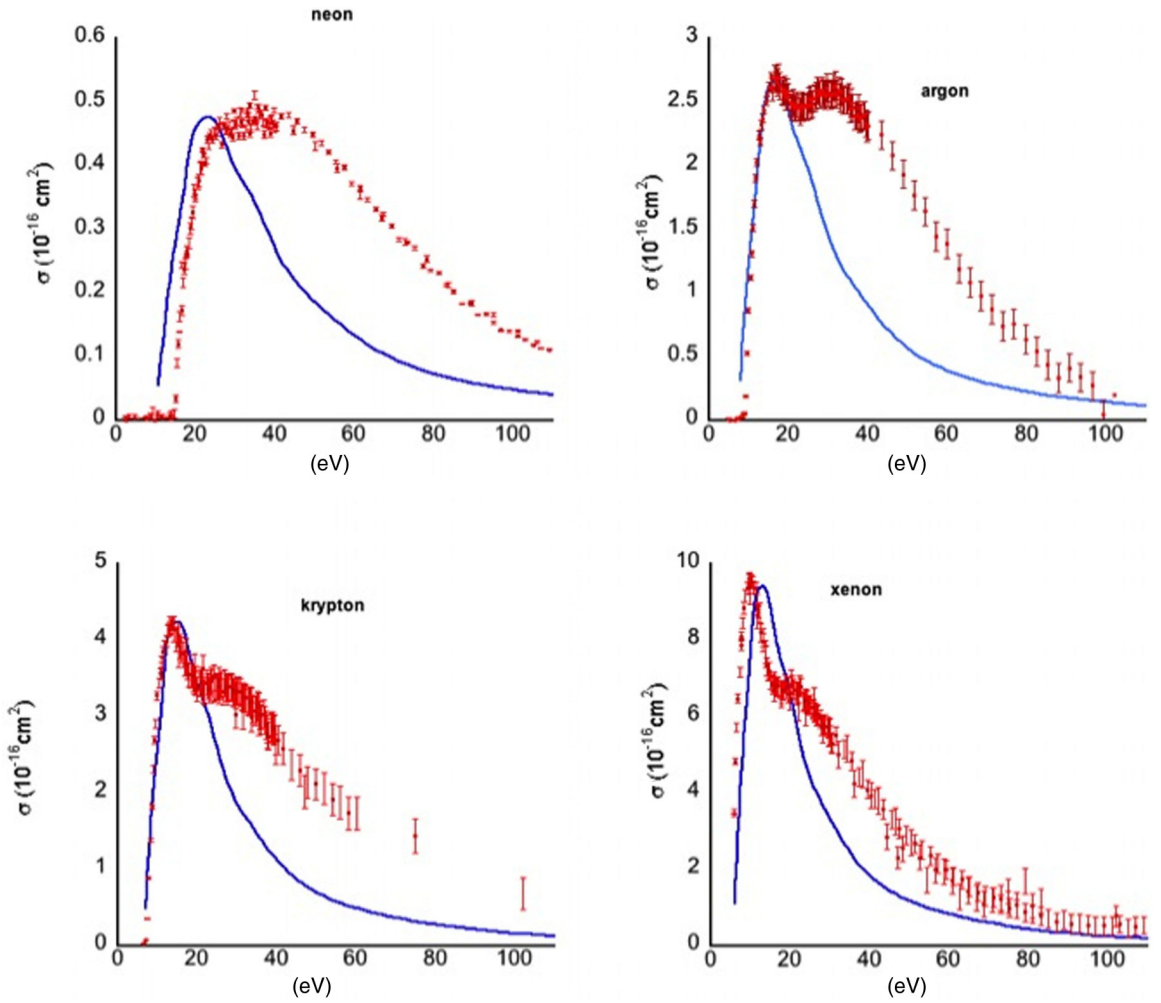

FIG. 8. (Color online) The charge-exchange cross section for e^+ on neutral noble gases calculated using Eq. (17), compared with the experimental data of Refs. [35,36]; the calculations have been multiplied by a factor to give the best visual fit to experiment (0.4 for neon, 1.2 for argon, 1.5 for krypton, and 2.5 for xenon).

B. Argon

In a plasma where there are free electrons and ions in different charge states, an injected positron can only do one of three things: annihilate with a free or bound electron; capture an electron to form positronium, which eventually annihilates; or escape the plasma. The study of an argon plasma in all stages of ionization is relevant to the planning for the LIFE project at the Lawrence Livermore National Laboratory [37]. It would be an ideal candidate to try out our idea of using an intense positron beam as a probe of plasma conditions. For annihilation with a free electron the resulting 511-keV line would be Gaussian. However, the shape of the line resulting from the decay of both singlet and triplet Ps will depend on the charge-exchange cross section and thus implicitly on which state of which ion the electron was initially in [38–40]. For positronium formation in e^+ collisions with neutral argon we are fortunate to have high-quality experimental data with which to compare our scaling formula (17). Our results are shown in Fig. 8. The scaled cross section lies about 20% below experiment at its maximum and is less broad. This is well within the acceptable tolerance of the plasma simulation codes. We have used the scaling method to calculate the cross sections for neon, krypton, and xenon and found that, despite its simplicity, the method always returns the correct order of magnitude and indeed tends to give the correction position for the maximum.

The primary focus of this work is the study of positronium formation in plasmas where there are a large number of atoms, ions, and free electrons. We have been at pains to demonstrate that the annihilation collisions between free electrons and positrons would have a much smaller cross section than those corresponding to electron capture by a positron from a neutral atom or ion in the plasma. As well as capturing an electron, a positron impacting an atom could also annihilate with a bound electron. Gribakin and Ludlow [41] have considered the 2γ annihilation rate on atomic targets near the positronium formation threshold and have shown that close to this threshold the positron annihilation cross section is essentially identical to the para-Ps formation cross section. However the region where this would be valid is exceedingly small (of the order of meV's) and as we move away from threshold the positronium formation cross section rises steeply and would quickly swamp any threshold annihilation signal, e.g., for hydrogen at 0.2 eV above threshold both theory [17] and experiment [29] find the

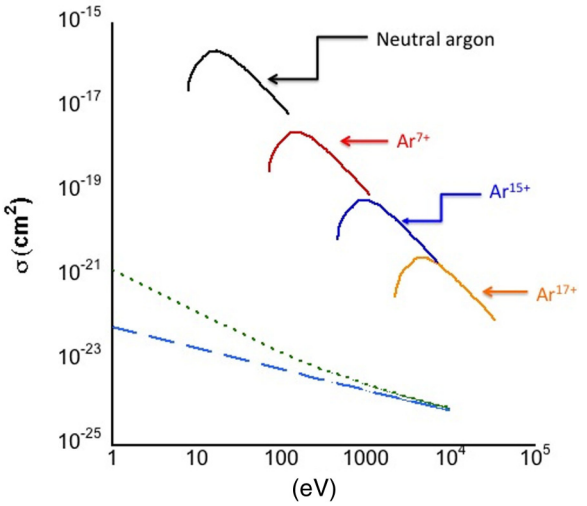

FIG. 9. (Color online) Charge-exchange cross sections from Eq. (17) for neutral argon and several different ionization states of argon, compared with the plane wave (dotted line) and Coulomb (dashed line) estimate for the in-flight annihilation cross section.

positronium formation cross section is 5 orders of magnitude bigger than the threshold cross sections given by Ref. [41]. The subhreshold annihilation signal is almost certainly beyond the limit of current experimental capabilities to measure and will certainly not be of significance in any plasma measurement.

For a plasma such as would be common in astrophysical conditions containing only hydrogen and helium, we can be confident that direct annihilation of the positron with a free or bound electron will be small compared with annihilation resulting from positronium formation. However, in the laboratory plasma of interest there will be a range of charge states and the higher the charge state the more positronium formation and annihilation with a bound electron will be suppressed as the positron will be discouraged by Coulomb repulsion from approaching the positively charged ion. Even so, Fig. 9 shows that positronium is expected to remain dominant over positron annihilation with a free electron [42]. It is reasonable also to assume that positron annihilation with a bound electron remains negligible compared with positronium formation as it is in hydrogen and helium.

It is worth noting that the charge-exchange cross section is appreciable only in a relatively narrow energy range, whose threshold and size will depend on the charge on the ion. Since the charge-exchange cross section will enter into any calculation of the γ-ray spectrum, the shape of the 511-keV line will implicitly depend on Z.

VI. CONCLUSIONS

Our work has been focused on finding a way to give a reasonable estimate of charge-exchange cross sections for positron collisions with atoms and ions. We have shown that the CTMC method works passably well for hydrogen and neutral cesium. We were able to deduce from our calculations that for hydrogen the electron is captured almost exclusively into the ground state, but for cesium much of the charge-exchange cross section is coming from capture into longer-lived states. Despite its successes, the CTMC method is difficult to employ for multielectron atoms and most probably has the wrong asymptotic behavior for ions; consequently we have looked for an alternative and introduced a simple scaling rule which appears to give a very good first estimate for both open and closed shell atoms. We applied it to positronium formation in positron-argon ion collisions and predicted that for all ionic states of the atom there would be a range of impact energies for which positronium formation would dominate over in-flight annihilation. This range would be of relatively narrow width with a sharp threshold, where both of these parameters would be Z dependent. This opens up the possibility of using positrons as a probe of ionized matter.

ACKNOWLEDGMENTS

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APPENDIX: A REMARK ON THE CONSERVATION LAWS IN PAIR PRODUCTION

We consider two cases:

(i) photon induced,

$$h\nu + A \rightarrow \bar{A} + 2A, \tag{A1}$$

(ii) particle induced,

$$A + A \rightarrow \bar{A} + 3A, \tag{A2}$$

where A denotes a particle and $\bar{A}$ its antiparticle, both of rest mass m_0. We wish to determine the threshold energy for both Eqs. (A1) and (A2). The most convenient way to do this is to work with four-vectors [43]. We use a formally Euclidean metric $g_{\mu,\nu} = \delta_{\mu,\nu}$ with an imaginary fourth component; e.g., the energy momentum vector for a particle with spatial momentum $\mathbf{p}$ and energy E is

$$\overleftrightarrow{\mathbf{p}} = \left(\mathbf{p}, i\frac{E}{c}\right). \tag{A3}$$

Note that the same equation holds for a photon moving in the direction of the unit vector, $\mathbf{e}$, whose four-vector is

$$\overleftrightarrow{\mathbf{p}}_\nu = \frac{h\nu}{c}(\mathbf{e}, i), \tag{A4}$$

where this vector has zero norm, i.e., $\overleftrightarrow{\mathbf{p}}_\nu \cdot \overleftrightarrow{\mathbf{p}}_\nu = 0$ in the Minkowski space. Let us first consider the photon-induced process, Eq. (A1). In the laboratory frame we assume that A is initially at rest so its four-vector will be $\overleftrightarrow{\mathbf{P}}_\mathbf{A} = (\mathbf{0}, im_0c)$, while for the photon entering along the z axis we have

$$\overleftrightarrow{\mathbf{p}}_\nu = \frac{E}{c}(\hat{\mathbf{k}}, i).$$

The total four-momentum before the collision is

$$\overleftrightarrow{\mathbf{P}}_{\text{total}} = \left(\frac{E}{c}\hat{\mathbf{k}}, i\left(m_0 c + \frac{E}{c}\right)\right).$$

Now the quantity

$$\begin{aligned}(\overleftrightarrow{\mathbf{P}}_{\text{total}})^2 &= \overleftrightarrow{\mathbf{p}}_{\nu}^{\,2} + \overleftrightarrow{\mathbf{P}}_{A}^{\,2} + 2\overleftrightarrow{\mathbf{P}}_{A}\cdot\overleftrightarrow{\mathbf{p}}_{\nu} \\ &= -(m_0 c)^2 - 2m_0 E \end{aligned} \tag{A5}$$

is Lorentz invariant and conserved; so after the collision it must be the same in the center-of-mass frame of the three particles. At threshold all three particles must be at rest in the center-of-mass frame. This minimizes the energy and is consistent with the requirement that the total spatial momentum must be zero in the center-of-mass frame. The square of the energy momentum four-vector is thus

$$(0,0,0,3(im_0 c))^2 = -9m_0^2 c^2. \tag{A6}$$

Then, combining Eq. (A6) with Eq. (A5), we have

$$\begin{aligned} -(m_0 c)^2 - 2m_0 E^{\text{photon}}_{\text{threshold}} &= -9(m_0 c)^2 \\ \Rightarrow E^{\text{photon}}_{\text{threshold}} &= 4(m_0 c^2). \end{aligned} \tag{A7}$$

Thus the photon needs to have a minimum energy of 2.044 MeV to create an electron-positron pair and a minimum energy of 3.76 GeV to create a proton-antiproton pair. For our second case we can repeat the analysis to find

$$E^{\text{particle}}_{\text{threshold}} = 6m_0 c^2. \tag{A8}$$

Thus the kinetic energy of an incoming electron needs to be greater than 3.066 MeV to create an electron-positron pair and we need a minimum proton impact energy of 5.64 GeV to create a proton-antiproton pair. Note that while the threshold energy for the particle case is greater, the cross section will also be greater once this energy is exceeded. The difference between a real photon and a virtual photon is a factor c^2 in the cross section. Finally if we consider pair production from a massive particle, such as a gold nucleus, assumed initially at rest, because of its massive size we may assume that its velocity in the laboratory will be very much less than c [43], so

$$\begin{aligned} \gamma Mc^2 &\approx \frac{1}{2}MV^2, \\ h\nu &= 2mc^2 + Mc(\gamma - 1) \\ &\approx 2m_0 c^2 + \frac{1}{2}MV^2, \\ \frac{h\nu}{c} &= MV, \end{aligned}$$

hence

$$h\nu = 2m_0 c^2 + \frac{1}{2}\frac{h^2\nu^2}{Mc^2}. \tag{A9}$$

For $Mc^2 \gg 1$ we can neglect the second term on the right-hand side of Eq. (A9) and the threshold energy for pair production off a massive particle is approximately $2m_0 c^2$. Further, the excess energy over threshold will be carried off as the kinetic energies of the electron and positron.

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