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Positronium Formation from positron impact on hydrogen and helium targets

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Disclaimer

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Charge exchange cross sections are presented for collisions of positrons and protons with hydrogen, neutral and singly ionized helium targets, using a variant of the classical trajectory monte carlo (CTMC) approach An extended error analysis is presented Good agreement with available experiment is found and the charge exchange cross section for positron on He^+ predicted.

Keywords: charge exchange, plasma, positronium

I. BACKGROUND:

The understanding of positron processes is an area of heightened interest in many branches of physics. In particular the significance of these has long been recognized in astrophysics. Positrons are produced at a tremendous rate at the center of the galaxy; estimates from studies of the 511keV gamma ray line suggests a rate of $\approx 10^{43} e^+/s$ [1]. Despite 30 years of intense effort the main source of these positrons has not been identified, for a recent review see [2, 3]. Further a knowledge of the ratio of the singlet state and triplet state photon fluxes would be a valuable diagnostic for understanding the physical conditions in a wide range of astrophysical sources, such as type Ia supernovae, microquasars, and x-ray binaries [2, 4]; a direct observation of positronium would be an important contribution to the physical understanding of jets escaping from quasars into the interstellar medium [5]; a study of 3γ versus 2γ emission would allow the determination of the temperature and density of the plasma in solar flares [6]. It is only recently that experimental progress has been made towards the goal of producing intense beams of positrons in the laboratory; Chen and her collaborators [7, 8] have succeeded in producing record amounts of positrons (they estimate 1 million particles per laser shot) and positrons have been observed in experiments by firing wakefield accelerated electrons into solid targets [9]. These new laser driver approaches open up the possibility that super intense positron sources will become a reality in the near future and consequently could be used as diagnostic tools and for the performance of significant experiments. Our own particular interest is in the possibility of using positronium formation as a probe of plasma properties and studying the positronium fraction in laboratory produced plasmas [4, 10, 11]. In astrophysical situations the plasmas of interest consist of hydrogen and helium atoms and ions, in this paper we will focus on positron collisions with neutral hydrogen and helium as well as with singly ionized helium. Our goal is to produce cross sections of sufficient accuracy which could be used in modeling of positronium formation in collisions between positrons and atoms or ions. We are fortunate to have available high quality charge exchange cross sectional experimental data for positron-neutral atom collisions[12] but there are no experiments for collisions between positrons and ions. Our approach has been to use the well known classical trajectory Monte Carlo approach for both the positron and proton projectiles Our strategy is to bench mark our theoretical approach for proton impact charge exchange before applying it to the equivalent positron process. Our approach has been to use the well known classical trajectory Mone Carlo method for both the positron and proton projectiles.

II. CLASSICAL TRAJECTORY MONTE APPROACH

The CTMC approach,[13–16] 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 [17] showed that the quantum mechanical probability distribution in momentum space for the n^{th} level of the hydrogen atom is given, in atomic units, by

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

is equal to

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

$p_n^2 = 2|E_n|$ and the identical distribution follows from the classical microcanonical distribution [13].

The classical nature of the CTMC approach means that there is capture into all states of the positronium with no account being taken of the discrete nature of the energy levels 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 [13, 18].

III. SOURCES OF ERROR

There are three main sources of error inherent in the CTMC method: (i) the error due to beginning and ending each simulated scattering event (or "run") with the projectile 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) 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, γ and ϵ, while (iii) can only be reduced by increasing the number of runs that our program cycles through for each incident energy.

IV. ERROR PARAMETERS γ AND ϵ

The value of the input parameter γ is approximately the ratio of the major diameter of the target atom to the initial distance between projectile and target. Its value is selected by the user and determines the starting and ending time of each run through the relationships

$$\gamma = \frac{|Z_eZ_n|}{E_iD_i(t_-)} = \frac{|Z_pZ_e|}{E_fD_f(t_+)} \tag{2}$$

defined in ([14]), where Z_p, Z_e, and Z_n are the charges of the projectile, target electron, and target nucleus, respectively; E_i and E_f are the binding energies of the initially bound target atom, and the finally bound "atom" resulting from the charge transfer; $D_i(t_-)$ is the initial distance between the CM of projectile and target atom at the beginning of the run; and $D_f(t_+)$ is the final distance between projectile and nucleus at the end of the run. Since the Coloumb interaction before time t_- and after time t_+ is neglected, it would seem that the smaller the choice of γ, the more accurate our simulation will be. However, as we shrink γ, we will need more steps in the numerical integration (assuming constant step-size), and thus the build up of error due to the finite step-size of the Runge-Kutta method becomes unmanageable. So we cannot just make γ as small as we wish–we must find a combination of both γ and ϵ that minimizes error.

The second error parameter, ϵ, determines the step length of the numerical integration, Δt, through the following relationship:

$$\frac{\epsilon^2}{(\Delta t)^2} = \left[\left(\frac{v}{r}\right)^2 + \frac{\epsilon}{2}\left|\frac{\dot{\mathbf{v}}}{r}\right|\right] \tag{3}$$

where v and r are the relative velocity and distance between two particles. Since there are three particles under consideration, Δt is actually computed by combining the above expressions for each two-particle interaction. It is worth noting that the step size varies with the product of the charges Z_p, Z_n. For a fixed value of ϵ, the step size will be smaller when the charge on either particle is increased, consequently finite step size problem will be more if either charge is greater than 1. We measure these errors by measuring how badly the program violates conservation of energy. This is done by evaluating the total energy of all three particles at the beginning and end of each run. There are four quantities of interest here: the actual initial energy of all particles (E_i); the initial energy neglecting the interaction between the projectile and target ($E_{i,mod}$); the actual final energy of all particles (E_f); and the final energy neglecting the interaction between the new atom and the nucleus–in the case of capture–($E_{f,mod}$). Each of these four quantities is evaluated for each event. We can measure the error due to starting and ending the collision at finite times by the differences $|E_i - E_{i,mod}|$ and $|E_f - E_{f,mod}|$. Likewise, we can measure the error due to finite step size in the numerical integration using the difference $|E_i - E_f|$; if the integration were 100% accurate, this difference would always be zero. We measure the average and the standard deviation of these differences each time the program is run. If for a given impact energy the error exceeds a certain limit, the result is not used. For positron projectiles, this limit is that the average of the absolute difference between E_i and E_f plus the standard deviation of this difference should be less than 35% of the impact energy of the positron:

$$\overline{|E_i - E_f|} + \sigma_{|E_i-E_f|} < .35T_{e^+} \tag{4}$$

Enforcing this inequality necessitated accepting quite large statistical errors at low energies for positron im-

pact processes It is well known from numerical treatments of the Kepler problem in celestial mechanics that standard integrating methods such as the Runge Kutta technique can give rise to similar violations in energy conservation[19]

V. STATISTICAL ERROR

The statistical error associated with the cross sections calculated by the CTMC program, is given by the binomial distribution ([13, 14]). Let us denote a particular event (such as charge transfer) by q, and the number of occurrences of that event by n_q. Then, letting n be the total number of runs, the statistical error associated with the cross section for q is given by

$$\sigma_q \left(\frac{n - n_q}{n_q \cdot n} \right)^{\frac{1}{2}} \tag{5}$$

where σ_q is the "experimental estimate" of the cross section for a particular property of the final state, q, and is defined by

$$\sigma_q = \frac{n_q}{n} \pi a_{max}^2 \tag{6}$$

where a_{max} is the radius beyond which event q no longer occurs. The maximum statistical error is then

$$\frac{1}{2\sqrt{n}} \pi a_{max}^2 \tag{7}$$

and occurs when $n_q = \frac{1}{2}n$. Figure 1 is a plot of how the error varies with n_q for a typical CTMC calculation of 10,000 runs.

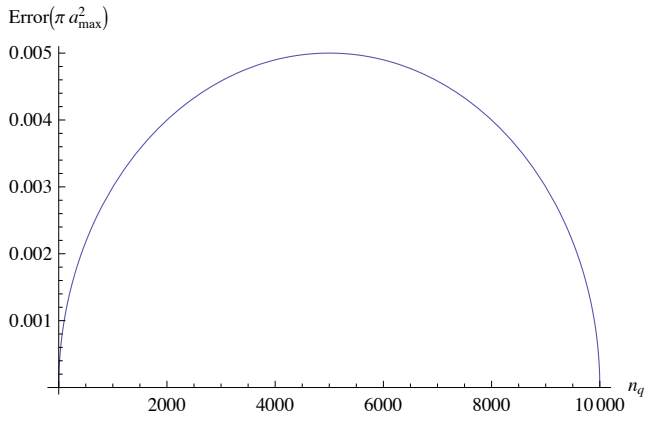

FIG. 1. *Statistical error as a function of n_q, with $n = 10,000$.*

VI. RESULTS

A. Hydrogen

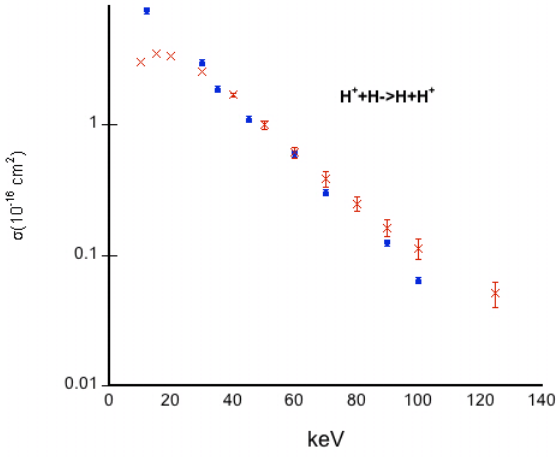

FIG. 2. *Charge exchange cross sections for proton collisions with neutral hydrogen:our theoretical calculations, CTMC, crosses, compared with the absolute experimental data of [20], solid circles*

Although the microcanonical distribution returns the quantum mechanical momentum distribution, the spatial distribution of the charge is less good. To correct for this Cohen[21] derived a new phase space distribution where the radial distribution is exact and the momentum distribution remains remains close to the quantum provided only that the target electron has a velocity($v_e < 9$). Using this distribution the ionization cross sections are improved but there is little change to the charge exchange results,[18, 22]. Since our interest here is exclusively with the latter we have used the "regular" microcanonical distributions in all our calculations. As we approach threshold the CTMC is at its weakest : as it does not recognize the sharp quantum thresholds and has no way of including tunneling effects and we need to chose a very large initial distance,(very small γ. We see that at its lowest energies our results peak and begin to fall away from experiment, we suspect that this is primarily due to the absence of tunneling in our calculations.[23]. The orbit of the positron will be fragile compared to than that of the much more massive proton and consequently one could reasonably assume that at the lowest energy it will not be able to get close enough for tunneling to become significant. Problems still exist in that because the approach will not recognize the correct quantum threshold. We have attempted to rectify this by shifting the origin i.e.we assume that the impact energy in the code E_code is related to the real impact energy by

$$E = E_{code} + E_{threshold}$$

where $E_{threshold}$ is the quantum threshold. Further as we approach threshold the problem we discussed in Section III of numerical violation of energy conservation, becomes more pronounced we tolerated a greater statistical error until such time the inequality in (4) was violated.

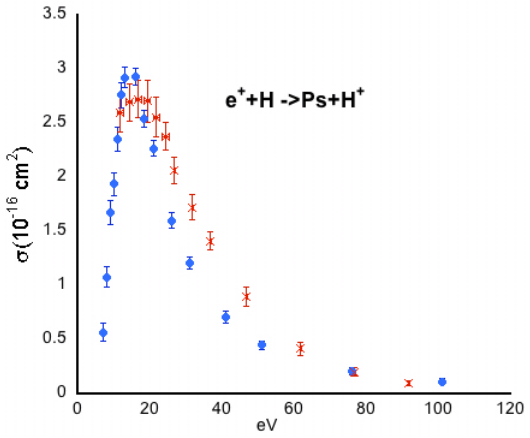

FIG. 3. *Charge exchange cross sections for positron collisions with neutral hydrogen:our threshold corrected CTMC calculations, crosses, compared with the absolute experimental data of [24], solid circles*

In Figure 3 we show our calculations compared with the experiment of Zhou *et al* [24]. Agreement is encouraging, in that we predict the absolute magnitude and position of the peak in the cross section correctly.

B. Helium

Following[25] we represented the potential $V(r)$ between the active electron and the He^+ by a model potential and by an effective Coulomb potential

$$V_{effective} = 1.688$$

and while the model potential of [25] gives a better momentum distribution the results are sufficiently close that we only show the cross sections calculated with the simpler effective charge potential. In Figure 4 we show a comparison between our CTMC calculation and experiment and while agreement is good for the range of values where a comparison is possible we note that our calculations exhibit the same qualitative behavior as we saw for hydrogen with a low energy peak so tunneling effects might well increase the cross section in this region. Our threshold corrected CTMC calculations are in good agreement with experiment for the positron case. Again the peak position is well predicted but the absolute magnitude at the peak is a little elevated above experiment

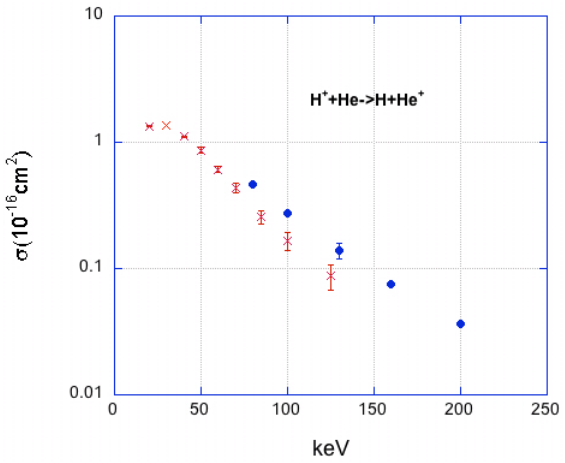

FIG. 4. *Charge exchange cross sections for proton collisions with neutral helium:,CTMC, crosses, compared with the absolute experimental data of [27], solid circles*

Our positron calculations are again threshold corrected.

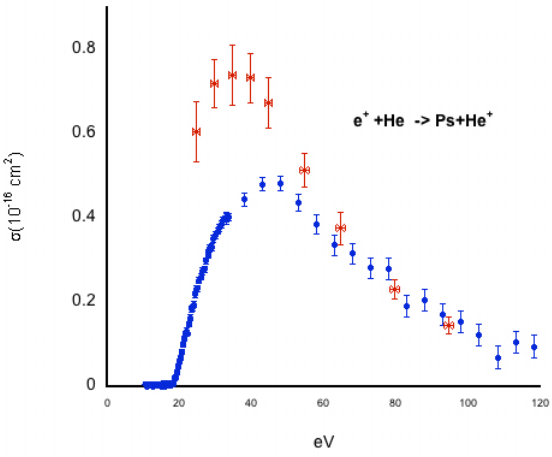

FIG. 5. *Positronium formation cross sections for positron collisions with neutral helium:threshold corrected CTMC, crosses, compared with the absolute experimental data of [12, 26] solid circles*

C. He^+

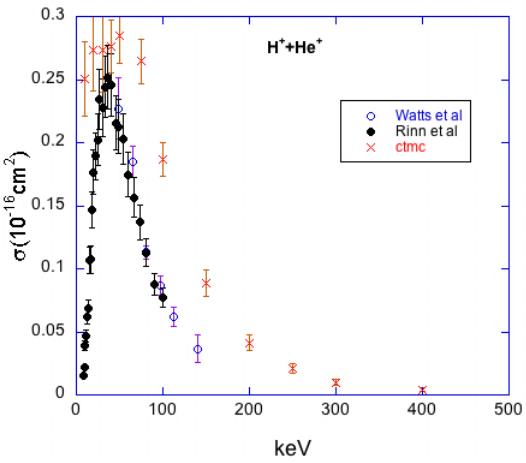

FIG. 6. *charge exchange cross sections for proton collisions with He^+:our theoretical calculations, CTMC, crosses, compared with the absolute experimental data of [28] solid circles and [29],open circles*

Finally we calculated the CTMC charge exchange cross section for singly ionized helium. In Figure 6 we show a comparison between the CTMC calculations and experiment for a proton on He^+. Both the position and the absolute magnitude of the peak in the experimental data is well represented, however the theoretical distribution is a little too broad. We were sufficiently encouraged that we calculated the threshold corrected CTMC for positron on He^+. Results are shown in Figure 7. There is no experimental data available however given the agreement we have found with other calculations in this paper it would seem likely that these results should be reasonably accurate and would be useful as part of a plasma simulation code which after all is our primary purpose.

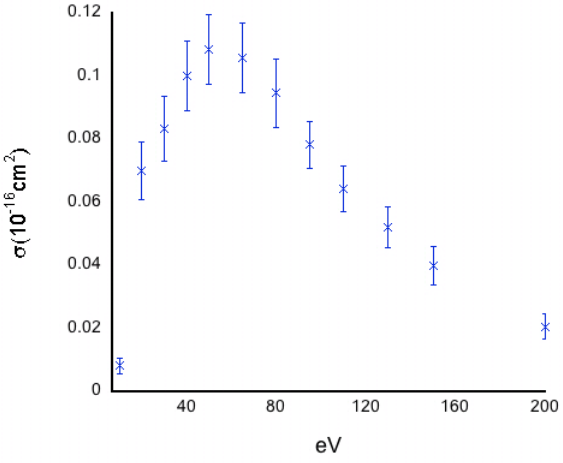

FIG. 7. *Positronium formation cross sections for positron collisions with He^+:in the CTMCqt, crosses,*

VII. CONCLUSIONS

We used the classical trajectory Monte Carlo method to calculate charge exchange cross sections for positron collisions with hydrogen, neutral and singly ionized helium targets with the ultimate purpose of including these results in plasma simulations. We benchmarked these results by comparison with experiment where available and by using the same method to calculate proton collisions with the same targets. Agreement was satisfactory in all cases The CTMC remains a useful way of estimating charge exchange cross sections, however it is important to keep careful track of the errors inherent in the code and it is misleading to present results without at least displaying the statistical errors. Further for the low energy positron collisions we found that the numerical integration using the standard 4^{th} order Runge Kutta gave rise to a numerical violation of energy conservation and the containment of this error placed a limit on how small our statistical error could be made. We hope to return to this problem latter.

VIII. ACKNOWLEDGMENTS

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