Positron scattering and ionization of neon atoms — theoretical investigations*

Harshit N. Kothari† and K. N. Joshipura

Department of Physics, Sardar Patel University, Vallabh Vidyanagar-388120, India

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Although positron scattering with inert gas atoms has been studied in theory as well as in experiment, there are discrepancies. The present work reports all the major total cross sections of e^+–neon scattering at incident energies above ionization threshold, originating from a complex potential formalism. Elastic and cumulative inelastic scatterings are treated in the complex spherical e^+–atom potential. Our total inelastic cross section includes positronium formation together with ionization and excitation channels in Ne. Because of the Ps formation channel it is difficult to separate out ionization cross sections from the total inelastic cross sections. An approximate method similar to electron–atom scattering has been applied to bifurcate ionization and cumulative excitation cross sections at energies from threshold to 2000 eV. Comparisons of present results with available data are made. An important outcome of this work is the relative contribution of different scattering processes, which we have shown by a bar-chart at the ionization peak.

Keywords: ionization cross sections, positron scattering, complex potential, total cross sections

PACC: 3485, 3485D, 3485B

1. Introduction

Apart from fundamental significance, the positron impact studies with matter have importance in the origin of astrophysical sources of annihilation radiation, as well as in the fields of medicine, characterization of materials,[1] and so on. Two phenomena that can occur only for positron collisions are annihilation (appreciable only for energies much less than 1 eV) and positronium (Ps) formation, the latter being important in positron–gas scattering processes. It is of interest to compare the positron scattering from a target with the scattering of electrons, for which more extensive theoretical and experimental data are available. We introduce first the different total cross sections (TCS) of the present relevance in e^+–neon scattering.

Total (complete) cross section labeled as $Q_{\rm T}$ is

$$Q_{\rm T}(E_{\rm i}) = Q_{\rm el}(E_{\rm i}) + Q_{\rm inel}(E_{\rm i}), \qquad (1)$$

where $Q_{\rm el}$ is the total elastic cross section and $Q_{\rm inel}$ is the total (cumulative) inelastic cross section at a given incident energy $E_{\rm i}$. The total inelastic contribution is comprised of Ps formation, electronic excitation and ionization of the target atom, and expressed as

$$Q_{\rm inel}(E_{\rm i}) = Q_{\rm Ps}(E_{\rm i}) + \sum Q_{\rm exc}(E_{\rm i}) + \sum Q_{\rm ion}(E_{\rm i}). \qquad (2)$$

The first term on the right-hand side of Eq. (2) is the positronium formation cross section which is large at low energies. The second term in Eq. (2) accounts for the sum of all accessible excitations in the target induced by the incident positrons. The third term indicates the sum of the total cross sections of all allowed (single, double, etc.) ionization processes. In the present energy range, which is from almost ionization threshold to 2000 eV, the first ionization is more dominant than double and higher ionizations. Therefore the last term will be denoted simply by $Q_{\rm ion}$.

Positron scattering with inert gas atoms has been studied in theory as well as in experiment by various research groups, but there are discrepancies among their results. Total cross sections ($Q_{\rm T}$) of e^+–neon system were measured in Refs. [2]–[6], but at an energy of 75 eV the $Q_{\rm T}$ data of Griffith *et al.*[4] are quite larger than the other measurements. Also the mea-

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†Corresponding author. E-mail: harshitkothari_85@yahoo.co.in

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sured values given in Refs. [2] and [3] differ in a range of 30–40 eV. The corresponding theoretical calculations of $Q_{\rm T}$ were carried out in Refs. [7]–[11]. Among these, the theoretical results in Ref. [7] are on higher side below 2000 eV. Discrepancies found among these data motivate us to carry out the present calculations at intermediate and high energies. The Ps-formation cross sections of all noble gases were measured by Marler *et al.*[1] and Laricchia *et al.*[12] They[1,12] have also measured direct (without Ps) ionization and total (including Ps) ionization cross sections for all inert gases. Bluhme *et al.*[13] measured total ionization cross sections for helium, neon and xenon atoms. Knudsen *et al.*[14] and Jacobsen *et al.*[15] measured single (direct) ionization cross sections of neon. Kara *et al.*[16] measured single and double ionization cross sections of neon. The excitation cross section and the ionization cross section of neon were measured by Mori and Sueoka.[17] Parcell *et al.*[8] also calculated positron impact excitation cross sections of neon for the first three states.

In this background on e^+–neon scattering, the present work reports all the major total cross sections at incident energies above ionization threshold, calculated by starting with complex potential formalism. We employ CSP-ic (Complex scattering potential-ionization contribution) method, used previously for electron scattering,[18−20] to deduce ionization cross sections from the corresponding inelastic cross sections.

2. Theory

The dynamics of e^+–neon scattering are treated presently in the complex potential formalism. For positron scattering the real part of the total complex potential $V(r, E_{\rm i})$ consists of static and polarization potentials while the imaginary part $V_{\rm abs}(r)$ accounts for the inelastic absorption effects. The potential components are derived from the target charge density of the atom, which is constructed from the wave functions of Bunge and Barrientos.[21] While the (repulsive) static potential $V_{\rm st}(r)$ is directly calculated from the target charge density, the polarization effects are included through the positron polarization potential $V_{\rm pol}(r)$ as given by Baluja and Jain.[11] The polarization potential is attractive and dynamic, i.e., energy-dependent. Thus at low-to-intermediate energies the static potential and the polarization potential tend to cancel each other and at high energies only the static potential dominates. The total complex potential consists of three potentials as shown below:

$$V(r, E_{\rm i}) = V_{\rm st}(r) + V_{\rm pol}(r) + {\rm i}V_{\rm abs}(r). \tag{3}$$

The polarization potential for positron scattering is defined below as per the detailed expression given in Ref. [11]:

$$V_{\rm pol}(r) = \begin{cases} V_{\rm corr}(r), & r \le r_{\rm c}, \\ -\dfrac{\alpha_{\rm d}}{2r^4}, & r \ge r_{\rm c}, \end{cases} \tag{4}$$

where $r_{\rm c}$ is the radial distance of the first crossing of the correlation term $V_{\rm corr}(r)$ and the asymptotic form $-\alpha_{\rm d}/2r^4$. The absorption potential $V_{\rm abs}(r)$ used presently to account for all inelastic channels with incident positrons was developed by Reid and Wadehra.[10] After generating all potential terms of Eq. (1), we treat it exactly in partial wave analysis by solving the first order differential equations for the real ($\delta_{\rm R}$) and the imaginary ($\delta_{\rm I}$) parts of the complex phase shift function. This is done in the variable phase approach of Ref. [22] as done in electron–atom/molecule scattering. The absorption potential $V_{\rm abs}$ depends on incident positron energy $E_{\rm i}$, target charge density $\rho(r)$, and energy gap Δ as per the expressions given in Ref. [10]. The energy-gap parameter Δ accounts for the energy conservation in the inelastic processes.[10] Basically it is a threshold such that if incident energy $E_{\rm i} \le \Delta$ then the $V_{\rm abs} = 0$ and neither excitation nor ionization can take place. Therefore, the choice of Δ proves to be crucial in obtaining the cross sections especially at low-to-intermediate energies. Now, if we fix the value of Δ at the positronium formation threshold ($E_{\rm Ps}$), the $V_{\rm abs}$ becomes unduly high near the peak of ionization cross section. On the other hand, if we keep Δ equal to ionization energy (21.56 eV) then even excitation channels are prevented at the lower energy end. Therefore, rather than choosing a fixed value, the Δ can be made to be increasing in a narrow range of incident energy, in a semi-empirical way. Previously in our electron scattering calculations we considered Δ to be $E_{\rm i}$-dependent as discussed in Refs. [18]–[20]. Presently also the energy dependence of the parameter Δ is assigned in a similar way to that in Ref. [18]. Specifically we express a simple functional dependence of Δ on $E_{\rm i}$ as follows:

$$\Delta(E_{\rm i}) = \Delta_{\rm min} + \beta(E_{\rm i} - \Delta_{\rm max}). \tag{5}$$

In this linear equation, we choose $\Delta_{\min} = 16.60$ eV which is the lowest excitation threshold for neon and $\Delta_{\max} = 19.08$ eV close to the ionization threshold (21.56 eV). Now, the energy $E_{\rm i}$ at which the $Q_{\rm inel}$ attains its maximum value is labeled as $E_{\rm p}$. Accordingly, the Δ is held constant at $\Delta_{\max}(= 19.08$ eV), at energies $E_{\rm i} \geq E_{\rm p}$. and hence we obtain $\beta = 0.0306$. In view of this argument our method becomes semi-empirical.

The above form of $\Delta(E_{\rm i})$ balances all aspects and also gives reasonably satisfactory cross sections in the present work. With the $V_{\rm abs}$ modified in this way, the cross sections $Q_{\rm el}$ and $Q_{\rm inel}$ are evaluated in a standard formulation.[18−20] The positronium formation and excitations dominate at lower energies. At incident energies well above $I = 21.56$ eV the ionization becomes more important than all other inelastic channels. Our aim is now to deduce the $Q_{\rm ion}$ from our calculated $Q_{\rm inel}$. There is no rigorous approach to projecting out ionization channel from the cumulative inelastic channels. Hence to find the contribution of $Q_{\rm ion}$ in $Q_{\rm inel}$ we introduce a method which we have previously[18−20] applied to electron impact on several atomic and molecular targets. In order to proceed along these lines we have to first obtain $Q_{\rm inel}$ without Ps-formation cross section. To this end we define the difference $Q_{\rm in} = Q_{\rm inel} - Q_{\rm Ps}$ and adopt the $Q_{\rm Ps}$ values from Marler *et al.*[1] Next we introduce the following ratio function, to bifurcate the ionization cross section from the $Q_{\rm in}$ cross section:

$$R(E_{\rm i}) = \frac{Q_{\rm ion}(E_{\rm i})}{Q_{\rm in}(E_{\rm i})}. \tag{6}$$

The ratio $R = 0$ when $E_{\rm i} \leq I$. Since the ionization corresponds to transitions in continuum the $Q_{\rm ion}$ is expected to dominate in the $Q_{\rm in}$ at high enough energy. Therefore, as in the case of electrons,[18−20] the present ratio function may also be expected to rise as $E_{\rm i}$ increases above I, and approach almost unity at high energies, such that

$$R(E_{\rm i}) = 0, \quad \text{for} \quad E_{\rm i} = I, \tag{7a}$$

$$R(E_{\rm i}) = R_p, \quad \text{for} \quad E_{\rm i} = E_{\rm p}, \tag{7b}$$

$$R(E_{\rm i}) = R', \quad \text{for} \quad E_{\rm i} \gg E_{\rm p}. \tag{7c}$$

In the present case of neon the input $R_{\rm p} = 0.8$ indicates 80% contribution of ionization in the cumulative inelastic scattering at the incident energy $E_{\rm i} = E_{\rm p}$. This in turn indicates the dominance of ionization channel over discrete electronic excitations. Now in Eq. (7c) the value of R' is nearly equal to 1 at high energies say $10E_{\rm p}$, the same as that in electron scattering. Next, for the actual calculation of $Q_{\rm ion}$ from our $Q_{\rm in}$ we need $R(E_{\rm i})$ as a continuous function of energy $E_{\rm i}$. Therefore, let us have

$$R(E_{\rm i}) = 1 - f(U) = 1 - C_1 \left[\frac{C_2}{U + a} + \frac{\ln U}{U}\right] \tag{8}$$

with

$$U = \frac{E_{\rm i}}{I}. \tag{9}$$

The reason for adopting a particular functional form of $f(U)$ equation (8) is discussed in our previous papers.[18−20] The two terms of $f(U)$ given in Eq. (8) is more appropriate since the 1st term in the square bracket ensures a better energy dependence at low and intermediate values of $E_{\rm i}$. Equation (8) involves dimensionless parameters C_1, C_2, and a, which reflect the target properties. The three conditions stated in Eqs. (7a)–(7c) are used to determine these three parameters in an iterative manner. Thus we first assume $a = 0$ and consider a two-parameter expression in Eq. (8). We employ therein the two conditions (7a) and (7b) to obtain C_1 and C_2. The two-parameter equation is then used to determine the value of R at a high energy $E_{\rm i} = 10E_{\rm p}$, and the same value is employed in Eq. (7c) to obtain a new set of three parameters C_1, C_2 and a. Having thus obtained the parameters, we calculate $Q_{\rm ion}$ from Eqs. (6) and (8), and therefore generate $R_{\rm p}$ value from these $Q_{\rm ion}$. The resulting $R_{\rm p}$ value is used next as an input to Eq. (7b) iteratively to finally calculate $Q_{\rm ion}$.

The target properties of interest, viz., ionization potential, polarizability, energy at the peak $E_{\rm p}$, cut-off polarization parameter ($r_{\rm c}$), the CSP-ic parameters a, C_1, and C_2 are shown in Table 1.

Table 1. Parameters of Ne atom, used in the present calculations.

ionization potential ($I_{\rm p}$)/eV[a]	21.564
Ps-formation threshold $E_{\rm Ps}$/eV	14.764
polarizability (a_0^3)	2.668
energy at the peak $E_{\rm p}$/eV	100
cut-off polarization parameter $r_{\rm c}$ (a_0)	2.457
a	12.263
C_1	–1.767
C_2	–7.503

[a] Ref. [23]

3. Results and discussion

In our recent paper[24] positron scattering on the lightest noble-gas atom He has been studied. Therefore presently we have focused our attention on e^+–Ne scattering. We have calculated here all the major total cross sections of positron impact with neon atoms from 25 eV to 2000 eV, by starting with the complex potential formulation. Using CSP-ic method we have calculated ionization cross sections and total excitation cross sections as discussed above. We now discuss the present results depicted in Fig. 1 along with comparisons, including those of electron scattering.

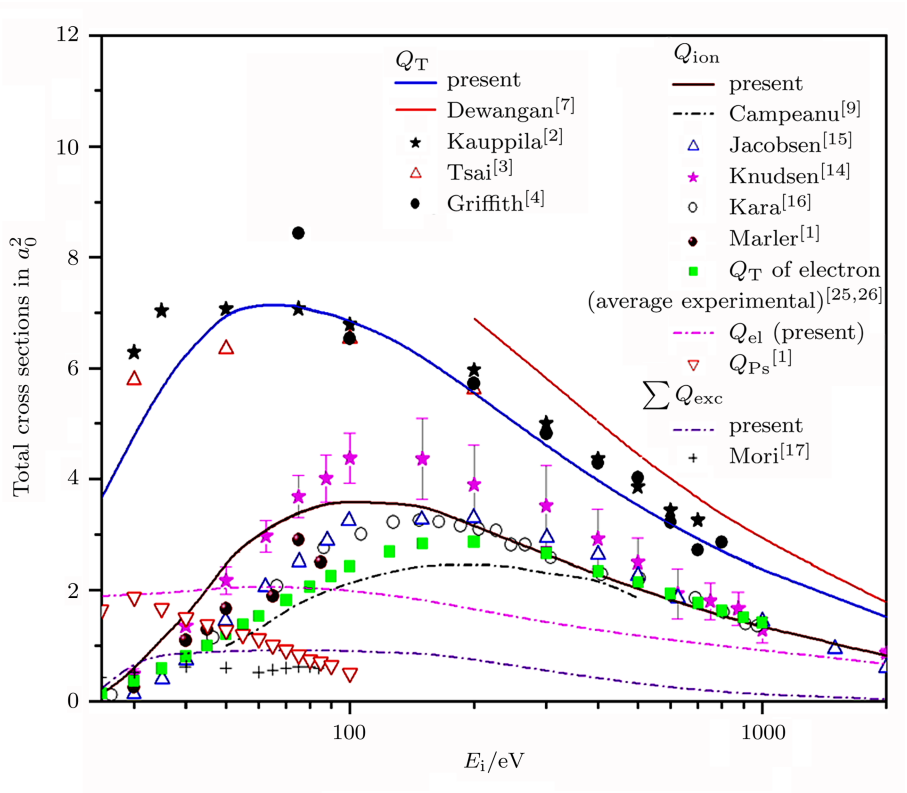


Fig. 1. All various total cross sections of neon by positron impact. Blue solid line: present Q_T; red solid line: Q_T by Dewangan;[7] Black star: Q_T by Kauppila *et al.*;[2] red triangle: Q_T by Tsai *et al.*;[3] black circle: Q_T by Griffith *et al.*;[4] wine solid line: present Q_{ion}; dash dot: Q_{ion} by Campaneu *et al.*;[9] blue triangle: Q_{ion} by Jacobsen *et al.*;[15] magneta star: Q_{ion} by Knudsen *et al.*;[14] circle: Q_{ion} by Kara *et al.*;[16] wine sphere: Q_{ion} by Marler *et al.*;[1] green square: average experimental[25,26] Q_{ion}; magneta dash dot: present Q_{el}; down red triangle: Q_{Ps} by Marler *et al.*;[1] violet dash dot: present $\sum Q_{exc}$; plus: Q_{exc} by Mori.[17]

In this figure the uppermost curve correspond to total positron cross sections Q_T of neon compared with other experimental[2−4] and theoretical results.[7] Due to opposite static and polarization interactions the total (complete) cross sections Q_T show a decreasing trend at low energies below 60 eV or so. Our Q_T values are in a good agreement with the experimental data of Refs. [2] and [3] above 40 eV, but towards lower energies some discrepancies are found. The theoretical results of Ref. [7] are higher than all other results displayed here. The results of Griffith *et al.*[4] are much higher at 75 eV, which is not expected. At 75 eV the data point of Griffith *et al.*[4] lies unexpectedly near the electron cross section (not shown). General shape and magnitude of the present Q_T curve are satisfactory.

Towards the lower portion of the figure we have depicted elastic, ionization and excitation results including a good comparison of magnitudes. Above the ionization peak, the single ionization cross sections of Knudsen *et al.*[14] are much higher than experimental as well as the present and the other theoretical

results. The present positron $Q_{\rm ion}$ show the maxima at 100 eV as against those of electron $Q_{\rm ion}$ near 200 eV. At low energy our $Q_{\rm ion}$ results are close to the data of Ref. [14] whereas the results of Jacobsen *et al.*[15] and Kara *et al.*[16] are in good agreement with our results after 150 eV. To compare the electron impact ionization cross sections with our present results of $Q_{\rm ion}$ for positrons, we have taken the average experimental electron impact data from the results of Refs. [25] and [26]. The theoretical $Q_{\rm ion}$ positron results of Campeanu *et al.*[9] are much lower than the present and all the other experimental results[1,14–16] and also lower than the average electron impact ionization cross sections.[25,26] It is noteworthy that towards lower energies, the positron ionization cross sections are higher than electron ionization cross sections for Ne. At high energies from 300 eV onwards our results tend to merge with all other experimental results of positron scattering and also of electron scattering, as expected.

We have also shown in Fig. 1 our present elastic cross sections for the e^+–Ne system. Our positron elastic cross sections have similar natures to graphical results of Baluja and Jain,[11] but the present values are lower than those of Parcell *et al.*[8] The compared data of Refs. [11] and [8] are not shown here to preserve clarity of graphs. The elastic cross sections for positrons are lower than the electron impact cross sections (not shown) at the lower energy end, because of the reasons already stated above, and also discussed in Ref. [27].

Finally our calculations also yield the total excitation cross sections $\sum Q_{\rm exc}$, and these are shown by the lowest curve in Fig. 1. Above 80 eV the excitation sum exceeds the Ps-formation cross sections. We have compared the present excitation sum with the data of Mori and Sueoka[17] who indirectly deduced the excitation cross sections for optically allowed transitions in Ne. The data[17] involving errors of 30% or more are lower than our present results. The data set in Ref. [8] for e^+ induced excitations to the first three states of Ne are also on the lower side of our excitation sum. Thus the present estimate on $\sum Q_{\rm exc}$ is an upper limit at their corresponding energies.

Tabulated numerical values of the present cross section data as functions of energy are available with the authors.

Now, it is of interest to assess the relative importance of different scattering channels in e^+–Ne interactions in the background of Ps formation. Therefore in our Fig. 2 we have shown a bar chart of all the present major total cross sections at energy equal to the peak of ionization i.e. 100 eV. Here the Ps-formation cross sections are taken from Ref. [1].

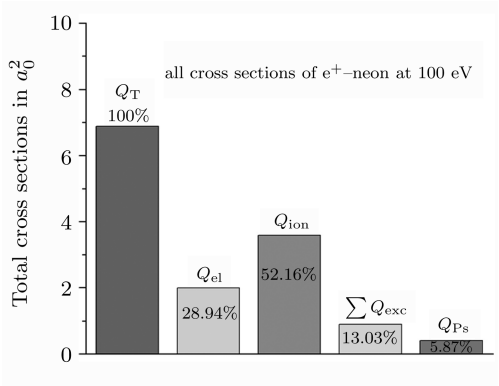


Fig. 2. All various total cross sections of e^+–neon at peak of ionization (100 eV).

4. Conclusions

The present work on positron–Ne scattering is motivated by discrepancies found in previous theoretical as well as experimental results of various studies. The work reported here is based on complex potential formulation, and it yields satisfactory values for all the important total cross sections of e^+–Ne scattering. The ionization contribution (CSP-ic) method previously applied to electrons,[18–20] is found to be successful presently for positrons in deducing $Q_{\rm ion}$ from $Q_{\rm in}$ for neon atoms, with due consideration to Ps formation, as in Eq. (6).

The results obtained from the present method are in reasonably good agreement with the available results for total cross sections and ionization cross sections, also this method has an advantage that we can also obtain total excitation cross sections as done presently. However, at low energies there are still differences among the present and other theoretical as well as experimental results. With the present cross section results it should be possible to infer average recommended data at intermediate and high energies. Further, as a follow up of our recent calculations on He in Ref. [24] and on Ne in the present paper, we plan to carry out the work on Ar and higher inert-gas atoms.

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