Projectile charge effects on the differential cross sections for the ionization of molecular nitrogen by positrons and electrons

G Purohit\textsuperscript{1,2} and D Kato\textsuperscript{1,3,4}

\textsuperscript{1}National Institute for Fusion Science, National Institutes of Natural Sciences 322-6 Oroshi-cho, Toki Gifu, 509-5292, Japan
\textsuperscript{2}Department of Physics, Sir Padampat Singhania University, Bhatewar, Udaipur-313601, India
\textsuperscript{3}Department of Fusion Science, SOKENDAI, 322-6 Oroshi-cho, Toki Gifu, 509-5292, Japan
\textsuperscript{4}Department of Advanced Energy Engineering, Kyushu University, Kasuga Fukuoka, 816-8580, Japan

E-mail: ghanshyam.purohit@spsu.ac.in

Received 10 March 2018, revised 16 April 2018
Accepted for publication 9 May 2018
Published 7 June 2018

Abstract
Triple differential cross sections (TDCSs) are reported for the positron and electron impact ionization of molecular nitrogen at a projectile energy of 250 eV. The TDCSs are calculated in the distorted wave Born approximation formalism using the orientation-averaged molecular orbitals. The present attempt is helpful for analyzing recent measurements (de Lucio and DuBois 2016 Phys. Rev. A \textbf{93} 032710) and studying the effect of projectile charge on the ionization of a molecular target. The TDCS trends are compared for positron and electron impact ionization in terms of binary and recoil intensities and binary lobe positions for different values of energy loss. The binary emission of electrons is enhanced for positron impact; however, nearly the same recoil emission is observed for positrons as well as electron impact. Significant discrepancies are observed in the measurements in terms of the relative binary intensity for positron and electron impact.

Keywords: TDCS, electron and positron impact ionization, molecular ionization, DWBA

(Some figures may appear in colour only in the online journal)

1. Introduction
The ionization of atoms and molecules by electron impact has been studied since the initial experimental work in [1], with special emphasis on the study of the triple differential cross section (TDCSs), which provide important information about the collision dynamics. Following this, the complete kinematics of the ionization process during and after the collision was learnt using powerful experimental techniques: cold target recoil-ion momentum spectroscopy (COLTRIM) [2] and recoil-ion momentum spectroscopy (RMS) [3]. Many of the experimental efforts have been on atomic targets, mostly inert gases [4]. For the last few years, there has been growing interest in investigating the collision dynamics of molecular targets. The closely spaced energy levels of different molecular states and the orientation of the molecule make it difficult to measure the TDCS, and it is also challenging for the theoretical models to describe molecular ionization due to the multi-center nature of the target wave functions. Despite this, TDCS studies have been done for molecular targets ranging from simple diatomic molecules to more complex ones, a few of which are listed as H$_2$ [5–7], N$_2$ [8–13], O$_2$ [14], H$_2$O [15–17], CH$_4$ [18–20] and HCOOH [21]. Complex molecules of biological interest, such as DNA analogues [22], pyrimidine [23], thymine [24], etc, have also been investigated. Distorted wave and time-dependent close coupling approaches have been used to calculate the cross sections for the molecular hydrogen target and both approaches have been successful in describing the features of TDCS [5, 25, 26]. Variants of the distorted wave formalism have been applied
for the electron impact ionization of various molecular targets (see [27] and the references cited) and a mixed degree of agreement has been achieved with the measurements, most of the time in good agreement with the binary lobe region and with certain discrepancies in the recoil scattering description [9].

Recently, ionization by antiparticle impact involving positrons has been studied experimentally as well as theoretically. Such types of study are helpful for understanding the similarities or differences between antiparticle–matter and particle–matter interactions, and are also helpful for obtaining certain information which cannot be obtained only by the study of electron impact processes [28, 29]. Differential studies with positrons are desirable for understanding the collision dynamics in comparison with projectiles, such as electrons or protons of the same energy, as well as to probe the effect of a projectile charge and mass on the collision dynamics. Due to technical problems regarding low signal intensities, there have been fewer positron impact differential cross section measurements in comparison to those measuring electron impact. To begin with, single differential [30] and double differential cross sections [31, 32] were reported for positron impact ionization. In a few later attempts, more single and double differential cross section results for the positron impact, and single as well as double ionization were obtained [33, 34]. Various theoretical efforts have been made to study the positron impact ionization of atomic hydrogen [35–38]. Structures in the triply and doubly differential ionization cross sections of atomic hydrogen have been identified [35] and the cross sections have been found to depend on the description of the three-body system [35, 36]. The ionization of atomic hydrogen by fast positrons has been studied in the presence of a laser field [37], and recently a study based on the two center approach to the fully differential positron impact ionization of hydrogen has been reported [38].

First, the triple differential cross sections were measured for the positron impact ionization of argon atoms in coincidence with both the outgoing particles moving in a forward direction [39]. The results of TDCS with a wider range of emission angles have been reported for argon atoms [40–42]. Theoretical efforts based on the distorted wave formalism tried to analyze the differential cross section trends of positron impact ionization for the measurements reported [43, 44]. A recent review details the progress and methods used in studying the inelastic interactions between positrons and atoms [45].

In the last decade, there has been increasing interest in the investigation of the positron impact collision dynamics of molecular targets, with emphasis on obtaining information which is inaccessible by the study of electron impact only. There have been a few attempts to measure the positron impact of fully differential cross sections for molecular targets. The triple differential study of the positron impact ionization of H₂ molecules has been reported for the forward emission of scattered and ejected particles [46, 47]. These efforts also verified the presence of a broad peak in the ejected electron spectrum attributed to the process referred to as electron capture to the continuum (ECC). Very recently, de Lucio and DuBois [12] reported the triple differential cross section measurements for the positron and electron impact ionization of nitrogen molecules at 250 eV projectile energy. Apart from the recent experimental study [12], no other study is available for positron- or electron-induced differential cross sections for N₂ molecules in the same kinematical conditions; however, electron impact TDCCs have been measured for nearly the same projectile energy [13]. It should be mentioned further that the total amount of cross sections has been calculated for the positron [48] and electron impact [49] ionization of N₂ molecules in the distorted wave Born approximation (DWBA) approach, and a reasonable degree of agreement was obtained with the measurements.

We report the TDCS results for the positron and electron impact ionization of nitrogen molecules at 250 eV projectile energy. We analyze the recent measurements [12] reported to study the projectile charge effect in the ionization of molecular nitrogen, following which no theoretical results are available for comparison, to the best of our knowledge. We also calculate and compare the electron impact TDCS for the ionization of N₂ molecules for the kinematical conditions of earlier measurements [13] in nearly the same energy regime (incident energy ≈300 eV) as the recent measurements [12]. The TDCCs have been calculated in the distorted wave Born approach using the orientation-averaged molecular orbital approximation, and the atomic units ( ħ = e = m_e = 1) were used.

2. Theory

The positron- and electron-induced TDCS may be written in the following form:

\[
\frac{d^5 \sigma}{d\Omega_1 d\Omega_2 dE_1} = (2\pi)^4 \sum_{av} |T(k_1, k_2, k_0)|^2.
\]  

(1)

A projectile with energy E_0 and momentum k_0 collides with the target molecule and produces scattered and ejected particles with energies E_1, E_2 and momenta k_1, k_2 respectively in the outgoing channel, which are observed in coincidence. The energy conservation E_0 = E_1 + E_2 + IP follows, where IP is the ionization potential of the target orbital. The transition matrix element (T) may be expressed in terms of the direct and exchange scattering amplitudes as:

\[
|T|^2 = |f_{dir}|^2 + |f_{ex}|^2 - Re(f_{dir}^* f_{ex})
\]  

(2)

where

\[
f_{dir} = \langle X_1(k_1, r_1) X_2(k_2, r_2) \frac{Z}{r_{12}} | \psi^{OA}(r_2) X_0(k_0, r_1) \rangle  
\]  

(3)

\[
f_{ex} = \langle X_1(k_1, r_1) X_2(k_2, r_1) \frac{Z}{r_{12}} | \psi^{OA}(r_2) X_2(k_0, r_1) \rangle
\]  

(4)

where Z = ±1 is the charge of the projectile (‘+’ for the positron and ‘−’ for the electron). The incident particle is described by the distorted wave \( X_0(k_0, r_1) \) and \( X_1(k_1, r_1) \); \( X_2(k_2, r_2) \) are the distorted wave functions used for the scattered and ejected particles respectively, and particles 1 and 2 are exchanged in the expression of the exchange amplitude (equation (4)). \( \psi^{OA}(r_2) \) is the initial bound state wave function.
for the molecular target, which is approximated as the orientation-averaged molecular orbital for the orbitals of the N₂ molecule. The molecular wave functions have been calculated using the density functional theory with the B3LYP/TZ2P basis set [50].

The initial state distorting potential representing the interaction between the projectile and the target molecular electrons constitutes the contribution from the molecular nuclei and a spherical symmetric potential obtained by averaging over all orientations using the B3LYP basis sets. The molecular charge density for the neutral molecule is obtained by

\[ \rho(r, R) = \sum_{k=1}^{m} n_k |\psi^{\Omega \lambda}(r, R)|^2 \]  

where ‘m’ is the number of orbitals in the molecule and ‘n_k’ is the occupation number of the orbital. The average radial charge density is obtained by averaging equation (5) over all orientations:

\[ \rho_{av}(r) = \langle \rho(r, R) \rangle. \]

The spherically symmetric static distorting potential is then obtained using the average radial charge density

\[ U_{el}(r_1) = \left( \int \frac{\rho_{av}(r) \, dr}{|r_1 - r|} \right). \]  

We also calculate the TDCS using the Coulomb potential in place of the spherically symmetric potential of equation (6) for the smallest ejected electron energy (E₂ = 6 eV) to see the differences in the trends of the TDCS.

As described above, the initial state static distorting potential is the sum of the electronic contribution and nuclear contribution, i.e., \( U_{static} = U_{el} + U_{nuc} \). The nuclear contribution (\( U_{nuc} \)) is obtained by placing the nuclear charge on a spherical cell with a radius equal to the distance of the nucleus from the center of mass. The final state distorted potential is generated in a similar way constituting the nuclear contribution and spherically symmetric potential generated in the field of a molecular ion. In addition to the static distorting potential, the exchange distorting potential of Furness and McCarthy [51], corrected by Riley and Truhlar [52], has been used to generate the total distorting potential:

\[ U_E(r) = 0.5[E_0 - U_{static}(r)] - [(E_0 - U_{static}(r))^2 + 4 \pi \, \rho(r)]^{1/2}. \]  

For the positron impact ionization there is no exchange amplitude \( f_{ee^*} \) and the following choices have been made. The distorted waves for the incident \( X_0(k_0, r_1) \) and scattered \( X_1(k_1, r_1) \) positrons are generated in the static potential of the molecular target, and the distorted waves for the ejected electron \( X_2(k_2, r_2) \) are generated in the static exchange potential of the molecular ion.

In order to see the effect of screening, the TDCSs have been calculated for the scattered particle in both the atomic potential and ionic potential; however, the ejected electron is treated in the potential of the residual ion in both cases. For the lowest ejected electron energy case (\( E_2 = 6 \) eV) the TDCSs have also been calculated by including the correlation-polarization potential \( V_{CP}(r) \) in the distorting potential. The correlation-polarization potential \( V_{CP}(r) \) is given as follows:

\[ V_{CP}(r) = V_{SR}^{corr}(r), \quad r \leq r_0 \]  
\[ = -\frac{\alpha_f}{2 \, r^2}, \quad r > r_0 \]  

where the fundamental form of the short-range correlation and long-range polarization potential has been approximated by means of the local density functional theory [53, 54]. \( \alpha_f \) is the dipole polarizability of the target and \( V_{SR}^{corr}(r) \) is the short-range correlation potential [53]. Point \( r_0 \) is the intersection of the short-range correlation and the long-range polarization potential, and we have ensured the smooth matching of potentials at \( r_0 \).

The Coulomb interaction between the two outgoing particles was treated using the Ward–Macek approximation [55], which has been found to give good agreement with the experimental data at lower energies and also reduces the computational difficulty [56].

The Ward–Macek factor is given by

\[ M_{ee} = N_{ee} |\tilde{F}_1(-i \, \lambda_3, 1, -2 \, i \, k_3, r_{3ave})|^2 \]  

where \( N_{ee} = \gamma \, e^\gamma - 1 \) is the Gamow factor, \( \gamma = -\frac{2\pi}{|k_1 - k_2|} \)

\[ \lambda_3 = -\frac{1}{|k_1 - k_2|} \quad \text{and} \quad r_{3ave} = \frac{\pi^2}{16 \, \varepsilon} \left( 1 + \frac{0.627}{\pi} \sqrt{\frac{\varepsilon}{\varepsilon}} \right)^2. \]  

\( \varepsilon \) is the total energy of the two exiting electrons. The sign of \( \gamma \) and \( \lambda_3 \) is changed for the PCI calculation of the positron impact.

The DWBA formalism, along with the orientation-averaged molecular orbital approximation, is capable of producing reliable TDCS results at the incident electron energy 250 eV used in the present study [11, 56]. The DWBA has been very successful at higher energies [9]; however, the DWBA with PCI effects has also been found successful at intermediate energies [56]. The DWBA is useful in describing the complex multi-center and multi-orientation problem of molecular ionization, as it can be applied for any energy and any size molecule, and effects such as the PCI also make it suitable for lower energies [56]. The orientation-averaged molecular orbital approximation used in the present investigation has been found to be successful for the symmetric molecular states (see [56] and references cited) and is useful for giving the first estimates for the positron impact ionization of molecular nitrogen; however, the calculation with the proper average over all orientations of the molecular target using the DWBA formalism is computationally challenging.

3. Results and discussion

The TDCS measurements for the positron impact ionization of nitrogen molecules were reported for the first time in [12].
The measurements of electron impact TDCSs have also been reported for the same kinematical conditions, and the TDCS trends obtained through experimental study of the positron and electron ionization of nitrogen molecules have been compared in terms of the relative binary and recoil peak intensities and the relative positions of the binary peaks. We report the results of the TDCS for the positron and electron impact ionization of molecular nitrogen for the same kinematical conditions used in recent measurements [12]. The TDCSs have been calculated in the distorted wave Born approximation for the ionization taking place from the 3σg orbital of N2.

The TDCS results are presented at a projectile energy of 250 eV for different average ejected electron energies at a scattering angle of 3°, through which the TDCS information is obtained for the momentum transfer ranging from 0.27 to 0.44 a.u. The calculated TDCS have been compared with the corresponding measurements. The TDCS results are displayed for an ejected electron energy of 12.4 eV in figure 1. The solid curve in figure 1(a) is the plot for positron impact ionization and the solid curve in figure 1(b) is the plot for electron impact ionization; the scattered particle is treated in the ion potential in both cases. The dashed curves in both frames are for the scattered particles treated in the atom potential. The solid red circles (figure 1(a)) and solid black circles (figure 1(b)) are the experimental TDCS [12] for the positron and electron impact ionization respectively. The measurements have been normalized to the positron TDCS (the solid curve in figure 1(a)) in the binary peak region for the best visual fit while retaining relative normalization between the electron and positron impact. The binary and recoil regions are identified in the TDCS results, experimentally as well as theoretically. The binary peak positions observed in the theoretical TDCS for the positron as well as the electron case are shifted towards lower values of ejected electron angle in comparison to the measurements. It is observed that the binary electron emission is enhanced for the positron impact ionization, which is similar, as shown by the measurements. However, there are discrepancies between the theoretical results and measurements in the relative magnitude of the binary peak for the positron and electron case. The recoil emission of the electron is decreased for positron impact ionization in the calculations; in contrast to this, the measurements have a recoil peak intensity that is slightly higher for the positron impact case.

The TDCS results calculated at ejected electron energies of 6.0 eV and 24.7 eV are presented in figure 2. These calculations have been done at a scattering angle of 3° for a momentum transfer of 0.29 a.u. (figures 2(a)) and 0.42 a.u. (figure 2(b)). The calculated TDCS results have been compared with the fits to the individual data obtained by [12] for the best visual fit, while retaining relative normalization between the electron and positron impact. At the small momentum transfer case (figure 2(a)) a large recoil peak is observed for both the positron and electron impact ionization in the DWBA results, but still retaining the nature of the trends: an enhanced binary peak and a smaller recoil peak for positron impact. The positron recoil peak in the calculated results is slightly higher than the electron impact at a larger momentum transfer (figure 2(b)). The TDCS curves with and without PCI are plotted for both the electron and positron impact case, and the PCI has not been found to change the trends of the TDCS significantly with changes less than 1% (see the solid black and black dashed curves in figure 2(a)). For a higher momentum transfer (figure 2(b)), the recoil peaks for the positron and electron impact ionization are of nearly the same intensities, as also observed in the measurements. As seen previously, there is a certain discrepancy in the theoretical results and measurements in terms of the relative height.
of the binary peaks for positron and electron impact and also in terms of the position of the peaks.

We have also calculated the TDCS for the ionization of N₂ molecules using the Coulomb potential in place of the spherically symmetric potential of equation (6) and including the correlation-polarization potential in the distorting potential. We observe that using different forms of potential does not change the trends of the TDCS significantly for either electron or positron impact ionization. The main discrepancy in the relative magnitude of the binary peak for the electron and positron impact still remains the same. Changes in the magnitude of the TDCS are observed, and the plots including different forms of potentials are presented in figure 3 for the lowest amount of ejected electron energy used in the present study (E₂ = 6 eV). The three outer 3σ₃g, 1π₃u and 2σ₃u valence orbitals of the nitrogen molecules have very near ionization potential values. We have calculated the TDCS for the contribution from these individual orbitals at an ejected electron energy of 12.4 eV (figures 4(a), (b)) and 6.0 eV (figures 4(c), (d)). We observe that the major contribution to the TDCS for both the electron and positron impact is from the 3σ₃g orbital. The TDCS calculated for the 2π₃u orbital has a larger binary peak and a smaller recoil peak; however, both
the $3\sigma_g$, $1\pi_u$ orbital TDCSs have a larger recoil and smaller binary peak ratio.

The discrepancies in the binary peak positions and the intensities of the binary and recoil lobes are better visualized through the comparison shown in figure 5, between the theoretical results and the measurements. The direction of the binary lobes for the 250 eV positron and electron ionization of molecular nitrogen are plotted as a function of momentum transfer in figure 5(a). The momentum transfer considered ranges from 0.27 a.u. to 0.44 a.u. corresponding to the various energy loss cases considered in the measurements [12]. The solid blue triangles and solid red circles are the experimental positions of the binary lobes for electron impact and positron impact respectively. The solid red line and blue dashed line are the binary positions observed by present calculations for positron and electron impact respectively. The black dotted line is the binary peak position calculated according to the kinematic conditions. An addition of a 10° angle has been made in the theoretical binary peak positions for better comparison with the measurements. The binary peak positions in the measurements are shifted towards higher values of ejected electron angle in comparison to the directions predicted by the theoretical results. The binary peak in the measurements for electron impact is at a higher ejected electron angle in comparison to the positron impact except for a few cases; however the present theoretical results show that the binary lobe for positron impact is observed at higher ejected electron angles (the solid red line in figure 5(a)).

The experimental and theoretical values for the maximum binary and recoil intensities are also compared as a function of momentum transfer in figure 5(b). Both the experiments and theoretical results show the increased binary emission of electrons for positron impact ionization (the solid red triangles and solid red line); however, the theoretical
We have also calculated the TDCS for the electron impact ionization taking place from the $3\sigma_g$ orbital of the nitrogen molecule for the kinematical conditions of earlier measurements [13], following which there are no other theoretical results available for comparison to the best of our knowledge. The DWBA results with OAMO are reported for ejected electron energies of 10 eV (figures 6(a), (b)) and 18.4 eV (figures 6(c), (d)) and compared with the measurements [13]. The measurements have been normalized to the theoretical results for the best visual fit. The binary peak for all cases overestimates the experimental binary peak; however, the binary to recoil peak ratio improves at higher values of scattering angles. The experimental and theoretical peak positions agree reasonably well, except figure 6(c).

The differences in the trends of TDCS for the positron and electron impact ionization of the nitrogen molecules are mainly attributed to the exchange term in the Hamiltonian due to the charge of the projectile. For the electron case, there is the exchange in the elastic scattering in the incident channel, and for both the outgoing electrons as well. The exchange amplitude is calculated and included in the calculation of the TDCS. For the case of the positron impact, there is no exchange amplitude and the distorted waves for the positron are generated in the static potential of the nitrogen molecule; however, the distorted wave for the ejected electron is calculated in the static exchange potential of the molecular ion. The post collision interaction (PCI) is included using the WM factor for both the electron and positron impact cases; it has the opposite sign for the positron case due to the presence of positrons and electrons in the outgoing channel. The role of PCI has not been found significant for the kinematics of the present calculations for either the electron or the positron impact cases, so the exchange is the dominant effect responsible for the different trends of TDCS observed. The TDCS curves including PCI and without PCI are plotted in figure 2(a) for the smallest amount of ejected electron energy, showing that the inclusion of PCI does not make a significant change in the trends of the TDCS. We have calculated the TDCS using the atom potential as well as the ion potential for the scattered particle (figure 1) as the scattered particle is faster than the ejected electron in the kinematics used presently. The shift of the binary peak position towards a higher ejected electron angle and an increase of magnitude is observed for the TDCS calculated in the ion potential for the scattered particle.

The description of the fully differential cross section for the electron impact ionization of a molecular target is still an open problem and there are many unanswered questions. The theoretical formalism used to date is basically based on variants of the distorted wave approach using orientation-averaged methods to describe the molecular target states; only a few nonperturbative attempts have been made for the hydrogen molecule [25, 26]. The present attempt is able to describe the trends of TDCS for the positron and electron impact ionization of nitrogen molecules up to some extent with points of agreement and disagreement with the measurements. The prime disagreement lies in the relative magnitude of the binary peak for the electron impact and the peak.

Figure 5. (a) The binary lobe angles plotted as a function of momentum transfer. The solid red line and the blue dashed line present the DWBA results with an addition of $10^7$ for positron and electron impact respectively; black dotted line: results calculated from the kinematics; solid red circles: measurements [12] for positron impact; solid blue triangles: measurements [12] for electron impact. (b) The binary and recoil intensities plotted as a function of the momentum transfer; solid red curve and red dashed curve: theoretical binary and recoil intensities for positron impact; solid blue curve and blue dashed curve: theoretical binary and recoil intensities for electron impact; solid red triangles and hollow red triangles: experimental binary and recoil intensities for positron impact [12]; solid blue triangles and hollow blue triangles: experimental binary and recoil intensities for electron impact [12]. The measurements for the binary intensity have been normalized to the solid red curve for positron impact for the best visual fit, and the other measurements have been plotted retaining the relative normalization.

relative intensity of the binary peak for electron impact is not as low as that reported by the measurements (the solid blue line and solid blue triangles). The measurements also show a higher recoil emission of electrons for positron impact ionization (hollow solid circles), and the theoretical results show a slightly higher recoil peak intensity for electron impact for a smaller momentum transfer (dashed red line).
positions. Larger binary peaks are observed in the present calculations for the electron impact ionization, which disagree with the measurements\cite{12, 13}. The OAMO method used in the present study has been found to be successful for molecules such as H\textsubscript{2} and N\textsubscript{2}\cite{11, 55}, particularly at smaller momentum transfer conditions below unity. The results obtained for the kinematics of the present study have a large degree of disagreement, as described above. We have also calculated the TDCS using the Coulomb potential as well as the addition of the polarization potential in the distorting potential; however, the trends of the TDCS have not varied significantly. The TDCS has also been calculated to see its contribution from the ionization of the other valence orbitals of the nitrogen molecules; however, the relative binary peak intensity for positron and electron impact is not observed as in the measurements\cite{12}. The disagreement with the measurements in terms of binary to recoil peak ratio may be due to second order effects, particularly at lower ejected electron energies. The other possible reason for the large discrepancies may be the use of the orientation-averaged molecular orbital. The proper average (PA) over the orientation-dependent cross sections may be another option, and has recently been found to give better agreement with the measurements for the H\textsubscript{2}O molecules\cite{57}; however the computational cost of the proper average method is exceptionally high, requiring more than a thousand processors. Calculations in the second order Born approximation may also be tested in the future. In the absence of any other theoretical results for analysis of the measurements\cite{12, 13} and the large uncertainty in the measurements reported (the authors of \cite{12} have already cautioned about making comparisons in the absolute scale, and the authors of \cite{13} have mentioned the uncertainties), the present effort in the OAMO may give predictions of theoretical TDCSs and provoke further theoretical attempts with other forms of approximation, such as the PA, as well as considering the second order Born term.

Figure 6. The TDCS plotted as a function of the ejected electron angle for the electron impact ionization of the N\textsubscript{2} molecule. Solid curve: the DWBA results with OAMO; solid black circles: measurements\cite{13}. The measurements have been normalized to a solid curve for the best visual fit. The kinematics is displayed in each frame.
4. Conclusions

In conclusion, the present study gives an insight into the positron and electron impact interactions with molecular nitrogen and the effect of the exchange term in the Hamiltonian due to the sign of the projectile on the collision dynamics. The trends of the TDCCs are extracted as a function of the momentum transfer through various energy loss values. The effect of the reversal of the direction of the Coulomb field between the projectile and the molecular target is studied through the relative intensities of the binary lobe for positron and electron impact and the directions of the binary lobes. There are points of agreement and disagreement between the theoretical and experimental results with large discrepancies. Both the theory and measurements show the enhanced binary emission of electrons for positron impact ionization. Nearly the same recoil intensities for positron and electron impact are observed for the higher momentum transfer, both in the theoretical and experimental results. There are significant discrepancies in the relative magnitude of the binary lobes for the electron impact case. The binary lobe positions obtained by the theoretical results are shifted towards lower values of ejected electron angles in comparison to the experimental positions. Furthermore, the TDCCs have been calculated with different forms of interaction potential, and the TDCC contributions from other valence orbitals have also been investigated; however, the prime discrepancy of the overestimated binary peaks for electron impact has not been resolved. Future efforts with the second order distorted wave Born approximation and proper average may be useful to further investigate the trends of TDCCs for the N$_2$ molecules in comparison with the available measurements.

Acknowledgments

We wish to thank Dr Chuangang Ning for help in calculating the B3LYP basis sets. We also thank Prof Don Madison for useful suggestions. GP acknowledges the JSPS Long Term Fellowship AY 2017 (L17538) provided by the Japan Society for the Promotion of Science. GP also acknowledges the National Institute for Fusion Science (NIFS), Toki, Japan for providing hospitality, and Sir Padampat Singhania University (SPSU), Udaipur, India for providing sabbatical leave.

ORCID iDs

G Purohit @ https://orcid.org/0000-0002-4243-0071

References

[1] Ehhardt H, Schulz M, Tekaat T and Willmann K 1969 Phys. Rev. Lett. 22 89
[2] Dorner R, Mergel V, Jagutzki O, Spielberger L, Ulrich J, Moshammer R and Schmidt-Bocking H 2000 Phys. Rep. 330 95
[3] Ulrich J, Moshammer R, Dorner R, Jagutzki O, Mergel V, Schmidt-Bocking H and Spielberger L 1997 J. Phys. B: At. Mol. Opt. Phys. 30 2917
[4] Naja A, Staicu Casagrande E M, Lahmam-Bennani A, Stevensson M, Lohmann B, Dal Cappello C, Bartschat K, Kheifets A, Bray I and Fursa D V 2008 J. Phys. B: At. Mol. Opt. Phys. 41 085205
[5] Al-Hagan O, Kaiser C, Madison D H and Murray A J 2010 Nat. Phys. 6 59
[6] Sentfleben A, Pfueger T, Ren X, Al-Hagan O, Najjari B, Madison D, Dom A and Ulrich J 2010 J. Phys. B 43 081002
[7] Milne-Brownlie D S, Foster M, Gao J, Lohmann B and Madison D H 2006 Phys. Rev. Lett. 96 233201
[8] Hargreaves L R, Coyler C, Stevenson M A, Lohmann B, Al-Hagan O, Madison D H and Ning C 2009 Phys. Rev. A 80 062704
[9] Lahmam-Bennani A, Staicu Casagrande E M and Naja A 2009 J. Phys. B 42 235205
[10] Murray A J, Hussey M J, Bray I, Gao J and Madison D H 2006 J. Phys. B 39 3945
[11] Chaluvali H, Ozer Z N, Dogan M, Ning C, Colgan J and Madison D 2015 J. Phys. B: At. Mol. Opt. Phys. 48 155203
[12] de Lucia O G and DuBois R D 2016 Phys. Rev. A 93 032710
[13] Avaldi L, Camilloni R, Fainelli E and Stefani G 1992 J. Phys. B: At. Mol. Opt. Phys. 25 3551
[14] Yang J and Doering J P 2001 Phys. Rev. A 63 032717
[15] Nixon K L, Murray A J, Al-Hagan O, Madison D H and Ning C 2010 J. Phys. B 43 035201
[16] Kaiser C, Speiker D, Gao J, Hussey M, Murray A and Madison D H 2007 J. Phys. B 40 2563
[17] Fernández-Menchero L and Otranto S 2014 J. Phys. B: At. Mol. Opt. Phys. 47 035205
[18] Chaluvali H, Ning C G and Madison D H 2014 Phys. Rev. A 89 062712
[19] Nixon K L, Murray A J, Chaluvali H, Amami S, Madison D H and Ning C G 2012 J. Chem. Phys. 136 094302
[20] Fernández-Menchero L and Otranto S 2010 Phys. Rev. A 82 022712
[21] Colyer C J, Stevenson M A, Al-Hagan O, Madison D H, Ning C G and Lohmann B 2009 J. Phys. B: At. Mol. Opt. Phys. 42 235207
[22] Jones D B, Builith-Williams J D, Bellm S M, Chiari L, Chaluvali H, Madison D H, Ning C G, Lohmann B, Ingólfsson O and Brunger M J 2013 Chem. Phys. Lett. 572 32
[23] Builith-Williams J D, Bellm S M, Jones D B, Chaluvali H, Madison D H, Ning C G, Lohmann B and Brunger M J 2012 J. Chem. Phys. 136 024304
[24] Bellm S M, Coyler C J, Lohmann B and Champion C 2012 Phys. Rev. A 85 022710
[25] Colgan J, Pindzola M S, Robicheaux F, Kaiser C, Murray A J and Madison D H 2008 Phys. Rev. Lett. 101 233201
[26] Colgan J, Al-Hagan O, Madison D H, Kaiser C, Murray A J and Pindzola M S 2009 Phys. Rev. A 79 052704
[27] Ali E, Nixon K, Murray A J, Ning C G, Colgan J and Madison D 2015 Phys. Rev. A 92 042711
[28] Laricchia G, Armitage S, Kover A and Murtagh D J 2008 Adv. At. Mol. Opt. Phys. 56 1
[29] Mc Govern M, Asaafrao D, Mohammel J R, Whelan C T and Walters H R J 2009 Phys. Rev. A 79 042707
[30] Mojom J, Laricchia G, Charlton M, Jones G O and Kover A 1992 J. Phys. B: At. Mol. Opt. Phys. 25 L613
[31] Schmitt A, Ceryn U, Moller H, Rainh W and Weber M 1994 Phys. Rev. A 49 R5(R)
[32] DuBois R D, Doudna C, Lloyd C, Kahveci M, Khayyat K, Zhou Y and Madison D H 2001 J. Phys. B: At. Mol. Opt. Phys. 34 L783
[33] Santos A C F, Hasan A, Yates T and DuBois R D 2003 Phys. Rev. A 67 052708
[34] Santos A C F, Hasan A and DuBois R D 2004 Phys. Rev. A 69 032706
[35] Berakdar J and Klar H 1993 J. Phys. B: At. Mol. Opt. Phys. 26 3891
[36] Fiol J and Olson R E 2002 J. Phys. B: At. Mol. Opt. Phys. 35 1173
[37] Pan J, Li S-M and Berakdar J 2007 Opt. Lett. 32 585
[38] Kadyrov A S, Bailey J J, Bray I and Stelbovics A T 2014 Phys. Rev. A 89 012706
[39] Kover A, Laricchia G and Charlton M 1993 J. Phys. B: At. Mol. Opt. Phys. 26 L575
[40] de Lucio O G, Otranto S, Olson R E and DuBois R D 2010 Phys. Rev. Lett. 104 163201
[41] de Lucio O G, Gavin J and DuBois R D 2006 Phys. Rev. Lett. 97 243201
[42] Gavin J, de Lucio O G and DuBois R D 2017 Phys. Rev. A 95 062703
[43] Campeanu R I, Walters H R J and Whelan C T 2015 Eur. Phys. J. D 69 235

[44] Purohit G and Kato D 2017 Phys. Rev. A 96 042710
[45] DuBois R D 2016 J. Phys. B: At. Mol. Opt. Phys. 49 112002
[46] Kover A and Laricchia G 1998 Phys. Rev. Lett. 80 5309
[47] Arcidiacono C, Kover A and Laricchia G 2005 Phys. Rev. Lett. 95 223202
[48] Campeanu R I, Chis V, Nagy L and Stauffer A D 2004 Nucl. Instr. Meth. In Phys. Res. B 221 21
[49] Toth I, Campeanu R I, Chis V and Nagy L 2008 Eur. Phys. J. D 48 351
[50] Lee C, Yang W and Parr R G 1988 Phys. Rev. B 37 785
[51] Furness J B and McCarthy I E 1973 J. Phys. B 6 2280
[52] Riley M E and Truhlar D G 1975 J. Chem. Phys. 63 2182
[53] Padial N T and Norcross D W 1984 Phys. Rev. A 29 1742
[54] Perdew J P and Zunger A 1981 Phys. Rev. B 23 5048
[55] Ward S J and Macek J H 1994 Phys. Rev. A 49 1049
[56] Madison D H and Al-Hagan O 2010 J. At. Mol. Opt. Phys. 2010 367180
[57] Ren X, Amami S, Hossen K, Ali E, Ning C G, Colgan J, Madison D H and Dorn A 2017 Phys. Rev. A 95 022701