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A Theoretical Study for Excitation of Electrons Collides with Positive Nitrogen Ions

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Abstract:

Nitrogen ions, principally singly ionized nitrogen (N II) and doubly ionized nitrogen (N III), significantly affect different atomic, molecular, and astrophysical studies fields. as a result of their frequent occurrence in stellar atmospheres, interstellar media, and planetary nebulae, analysis of their spectral lines provides valuable details on environmental conditions such as temperature, density, and ionization states. This study indicated that N II and N III are excited by electron collisions for transition states. The Born-Bethe approximation was used to calculate the integral and differential cross-sections as well as the generalized oscillation strength. The results were agreed with other references in various transitions.

Key Word: Excitation, Nitrogen Ion, Born-Beth, Cross Section, Oscillator Strength

Introduction:

Singly-ionized nitrogen (N II) and doubly-ionized nitrogen (N III) have significant effects on astrophysical, atomic, and molecular physics (Yıldız & Gökçe, 2014). These ions are plentiful in stellar atmospheres, the interstellar medium, and planetary nebulae, and their spectral lines yield information on environmental characteristics like temperature, density, and ionization states (Stafford et al., 1994).

The study of N II and N III is necessary in fusion research and plasma diagnostics, where nitrogen is often used as a plasma contaminant or diagnostic element to monitor the characteristics of high-temperature environments (Z.-B. Chen, 2023). In the same way as carbon, nitrogen is one of the dominating chemical elements essential for life on our planet(Shen et al., 2018). As a result, nitrogen and its ions are of great focus in the contemporary world(Mahato et al., 2022; Tayal, 2011). Investigated the contributions of carbon and nitrogen originating from the cosmos, with their nitrogen data sourced mainly from N II measurements from spiral discs, post-star-burst galaxies, and H II regions of the galaxy at

the periphery(Henry et al., 2000). These results conform to (Rubin et al., 1998), who looked at the N+ region of the Orion Nebula concerned with its temperature variations using HST N II observations (Rubin et al., 1998).

Additionally, the improvements of various computational techniques, in particular the Hartree-Fock wave function method and the Bethe approximation (Musielok, 2014), led to the improvement of the calculations of the cross sections for excitation, transition probabilities, and the lifetimes of excited states of the N II and N III (Xiao-Zhi et al., 2007). Ions such advances have enabled great efficacy. All this progress in computing and experimental techniques has changed significantly in recent years in calculating the same method in our earlier things for calculating noble gases (Hassan & Khalaf, 2019). Phenomena, including earlier studies of lithium, significantly impacted theories of neutron stars (M. Abdul Hassan & A. Khalaf, 2019). In addition, it supplements the molecular structures studied recently on the atoms (Yassir & Khalaf, 2024), including the methane molecule. These advancements allow for improved modeling of electron transitions and particle interactions, enriching fundamental spectroscopic data and enhancing the accuracy of astrophysical models and plasma diagnostic applications(Z. Chen, 2024). This research is poised to deepen our understanding of nitrogen. This study aims to provide a detailed analysis of excitation cross-sections, transition probabilities, oscillator strengths, and lifetimes for selected excited states of N II and N III ions. These calculations are performed using advanced techniques, and the results are compared with available theoretical data. We hope this study will contribute to filling knowledge gaps regarding the atomic properties of nitrogen ions, thereby enhancing the reliability of scientific models in astrophysics and advanced plasma applications.

Theory:

In the excitation process of atoms by fast electrons, where they transition from the initial (i) state to the final (f) or excited state, the integral cross section is evaluated using the Born approximation. In this context, the generalized oscillator strength (GOS) plays a crucial role (Inokuti, 1971; Kim & Cheng, 1978) and can be expressed as follows:

$$\sigma_n^{Born} = \frac{4\pi a_0^2 R^2}{T E_n} \int_{(K_{min}a_0)^2}^{(K_{max}a_0)^2} f_n(K)\, d\, ln(Ka_0)^2 \tag{1}$$

$$f_n(K) = \frac{E_n}{R} \frac{\left|\left\langle f\left|\sum_j e^{i\vec{K}.\vec{r}_j}\right|i\right\rangle\right|^2}{(Ka_0)^2} \tag{2}$$

Where $f_n(K)$ is the generalized oscillator strength (GOS), E_n represents the excitation energy for the transition from the initial state to the final state, $\overrightarrow{K}$ is the momentum transfer, $a_0$is the Bohr radius, $\vec{r}_j$ is the position of the j^{th} Electron in the target, R is the Rydberg energy, and T is the incident electron's energy. The limits of the momentum transfer, K_{max} and K_{min} , are given by

$$(K_{min}a_0)^2 \approx \frac{E_n^2}{4TR} \equiv\ Q_{min} \tag{3}$$

$$(K_{max}a_0)^2 \approx \frac{4T}{R} \equiv\ Q_{max} \tag{4}$$

The Bethe cross section is the leading component of the approximated Born cross section and is expressed in terms of the parameters. $A_n$and $B_n$as follows:

$$\sigma_n = \frac{4\pi a_0^2 z^2}{T/R}\left[A_n \ln\left(\frac{T}{R}\right) + B_n\right] \quad (5)$$

$$A_n = f_n \, {}^{R}/_{E_n} \quad (6)$$

$$B_n = A_n \ln\frac{4R^2 Q_0}{E_n^2} \quad (7)$$

Where f_n is the optical oscillator strength and $Q_0$is the cutoff parameter, with Q_{min} and Q_{max}defining its limits. The total wavefunction, expressed as a Slater determinant, is given by(Tayal, 2008):

$$\psi = \Re(\emptyset_i \ldots \emptyset_f) \quad (8)$$

Where $\Re$ is the anti-symmetrizing factor, n is the number of electrons, and $\emptyset_i$ and $\emptyset_f$are the spin-orbitals (one-electron functions). It is assumed that the orbitals are orthogonal to each other, allowing the spin-orbitals to remain the same. In terms of the basis functions, the orbital $\emptyset_{n\ell}$Can be expanded as follows:

$$\emptyset_{n\ell} = \sum_i c_n^i \chi_{i\ell} \quad (9)$$

The one-electron functions have a radial part that is expressed in analytic form as a summation of Slater-type orbitals, given by(Hudson & Bell, 2005):

$$P_{n\ell} = \sum_{i=1}^{K} C_{in\ell} N_i r^{P_i} e^{-\xi_i r} \quad (10)$$

Where$C_{in\ell}$ is the expansion coefficient, and ξ is the orbital exponent.

$$N_i = \left(\frac{2(\xi_i)^{2P_i+1}}{(2P_i)!}\right) \quad (11)$$

Table I presents the Hartree-Fock wave functions for the 2p state and the wave functions for the 3d, 3s, 4d, and 4s states, taken from (Hudson & Bell, 2004). These wave functions correspond to the Hartree-Fock nitrogen ions N II calculations. Table II presents the Hartree-Fock wave functions for the 2p state and the wave functions for the 3d, 3s, 4d, 4s, and 5d states, also taken from (Corrégé & Hibbert, 2002). These wave functions correspond to the Hartree-Fock nitrogen ions N III calculations.

The radiative transition probability (sec^{-1})for the state (*f*) is given by(Zheng et al., 2000):

$$A_f = \sum_i A_{if} \quad (12)$$

$$A_{if} = \frac{1}{2}\,\alpha^3\,\frac{g_i}{g_f}\,\Delta E^2 f_{if} \quad (13)$$

Where $g_i$and g_fAre the statistical weight factors, and α is the fine structure constant. The lifetime of a state is given by:

$$\tau_f = \frac{1}{A_{if}} \quad (14)$$

Table 1: Orbital parameters for N II

Orbital	Power Of r	Orbital exponent	Expansion coefficient
2P	2	10.73127	0.53054
	2	4.15522	0.18887
	2	1.49966	0.33066
	2	1.02543	0.01355
3d	3	1.82592	0.02354
	3	0.77599	0.46059
	3	0.65024	0.53479
3s	1	5.69655	0.11825
	2	2.07460	-0.49585
	3	0.94717	1.09576
4d	3	2.13964	1.34081
	3	2.16613	-0.54915
	4	1.34164	0.44544
	4	0.81866	-0.70694
4s	1	2.38853	1.41548
	2	2.31023	-4.58360
	3	2.26604	3.80048
	4	1.10471	-0.70819

Table 2: Orbital parameters for N III

Orbital	Power Of r	Orbital Exponent	Expansion Coefficient
2P	2	2.42497	0.42629
	2	3.96654	0.10051
	2	1.88098	0.49912
	2	8.45838	0.00673
3d	3	0.80391	0.22080
	3	1.14127	0.79688
3s	3	0.57022	-0.00152
	3	1.23360	1.25036
	2	2.06530	-0.72535
	1	5.46414	0.15928
4d	3	2.61492	1.07915
	4	1.27775	-0.56038
4s	1	2.45545	0.76608
	2	2.18942	-2.54126
	3	1.20744	10.68445
	4	1.36397	-9.72325
5d	3	4.37432	0.58367
	4	0.98726	1.19603
	4	2.04106	-1.26420

Results and Discussions:

This study's primary focus is determining the nitrogen ion's cross sections and generalized oscillator strength. The cross sections for some potential excitation processes have been calculated, as the oscillator strength is the critical factor in predicting the cross sections for the excitation process of electrons that collide elastically with ions.

In Figure 1, the current work presents the integral cross section for the excitation of the nitrogen ion N II for a set of excitation states. All the calculated transitions have been compared with the theoretical study by(Ganas, 1980), which employed the Born approximation and represented the six-electron system by an independent-particle model in its calculations.

For the transition $2P^2 \rightarrow 2P\ 3S$, we observe that the agreement between our calculations and the theoretical results is excellent and closely follows the theoretical behavior. However, for the transition$2P^2 \rightarrow 2P\ 3d$, Our results show slight deviations from the theoretical predictions.

In the case of the transition $2P^2 \rightarrow 2P\ 4S$, The results are generally consistent with the theoretical predictions, except for the energy ranges from 10 to 30, where a discrepancy is noted. For the final transition $2P^2 \rightarrow 2P$ 4d, as mentioned earlier, due to the dependence of the cross-section on the oscillator strength, a difference between our calculations and the theoretical results, except for the final part, where complete agreement is achieved.

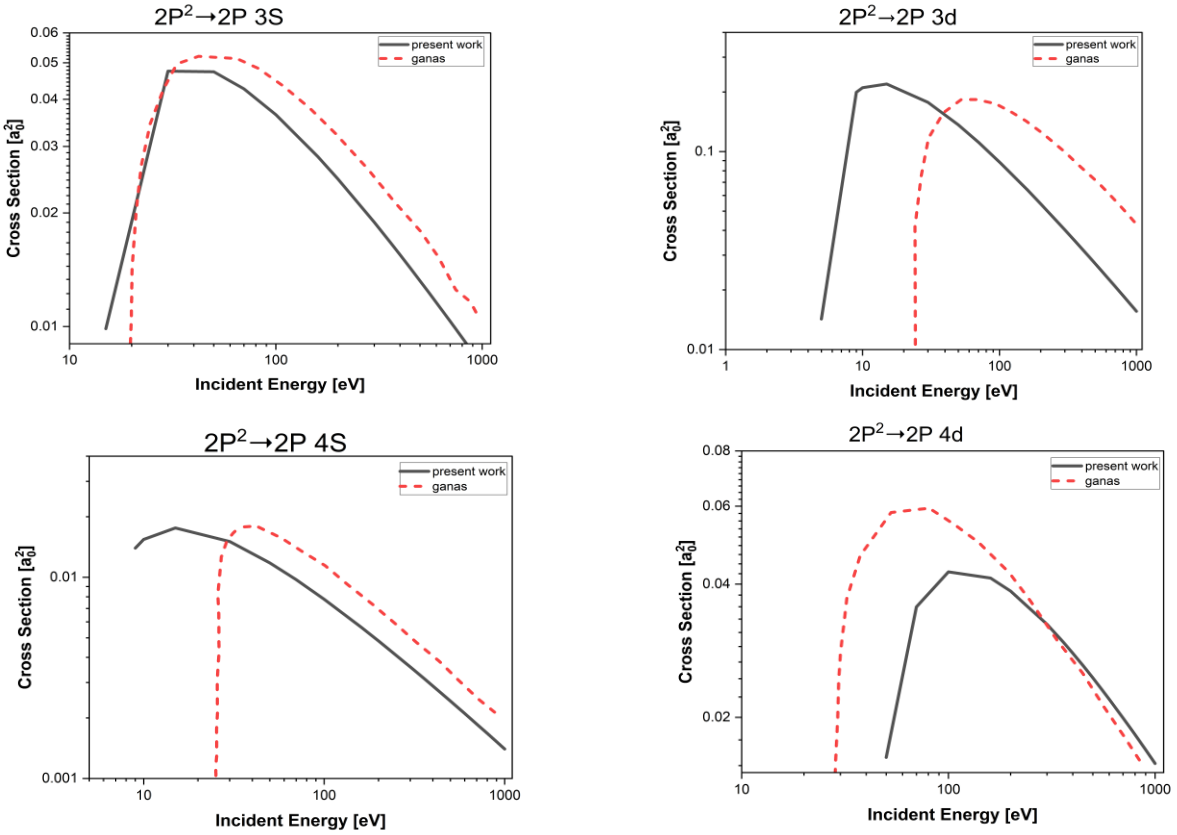

Figure 1: The Integral Excitation Cross Section for Electron Impact with N II for different transitions. the solid line in the present work and the short dashed line by (Ganas, 1980)

Figure 2 presents the integral cross section for the excitation of the nitrogen ion (N III) for a set of excitation states. All the calculated transitions have been compared with the theoretical study (Ganas, 1980), which employed the Born approximation and represented the Five-electron system by an independent-particle model in its calculations

The results for this transition $2p \rightarrow 2S^2 3S$ follow the same pattern as the theoretical predictions, with a discrepancy observed at the beginning of the graph in terms of energy. In another transition $2P \rightarrow 2S^2 3d$, we observe a slight difference between our results and the theoretical predictions; however, the function behaves similarly to the theoretical function. We note a similar behavior for this transition $2P \rightarrow 2S^2$ 4S as with the previous two. This is attributed to the slight difference in the oscillator strength. On the other hand, in a different transition $2P \rightarrow, 2S^2 4d$, our results and the theoretical predictions differ noticeably. This discrepancy is due to the value of the oscillator strength we found, which plays a crucial role in calculating the cross-section. Finally, the last transition, $2P \rightarrow 2S^2$ 5d, shows excellent agreement with the theoretical results, demonstrating a close match.

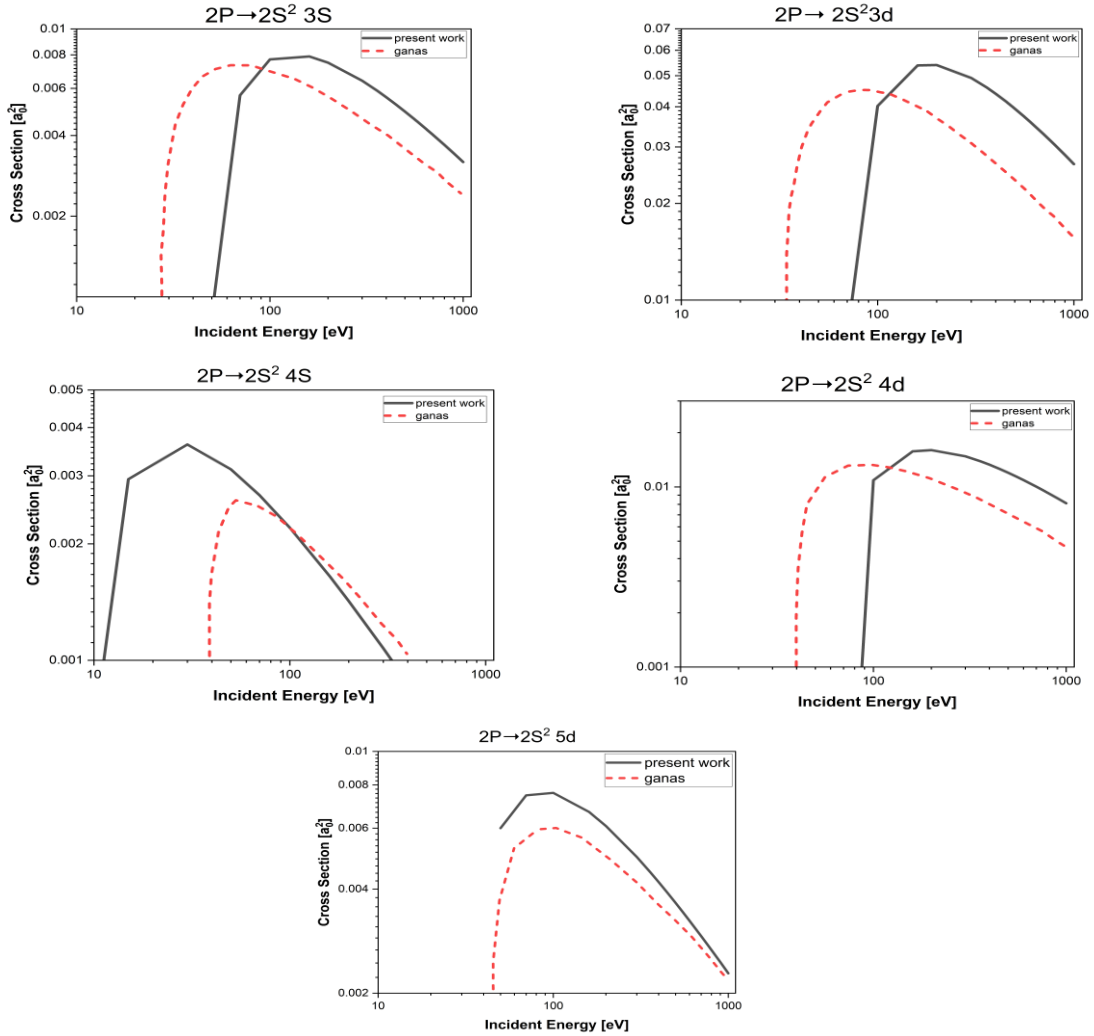

Figure 2: The Integral Excitation Cross Section for Electron Impact with N III for different transitions. The solid lines are present work and short dashed lines (Ganas, 1979)

As for the differential cross-section of the nitrogen ion, we did not find any previous studies for comparison to our knowledge. However, it is not suitable for comparison because the energy used in that study was 10 eV, while our calculations for the nitrogen ion N II range from 18 to 24 eV, and for the other ion N III, from 27 to 42 eV. Therefore, a comparison cannot be made, as it is evident from the energy range that it does not include the transitions we calculated.

Therefore, Figure 3 shows our calculations for the differential cross-section of the nitrogen ion (N II). Figure 4 shows the nitrogen ion (N III) calculations, using a kinetic energy range from 100 to 600 eV.

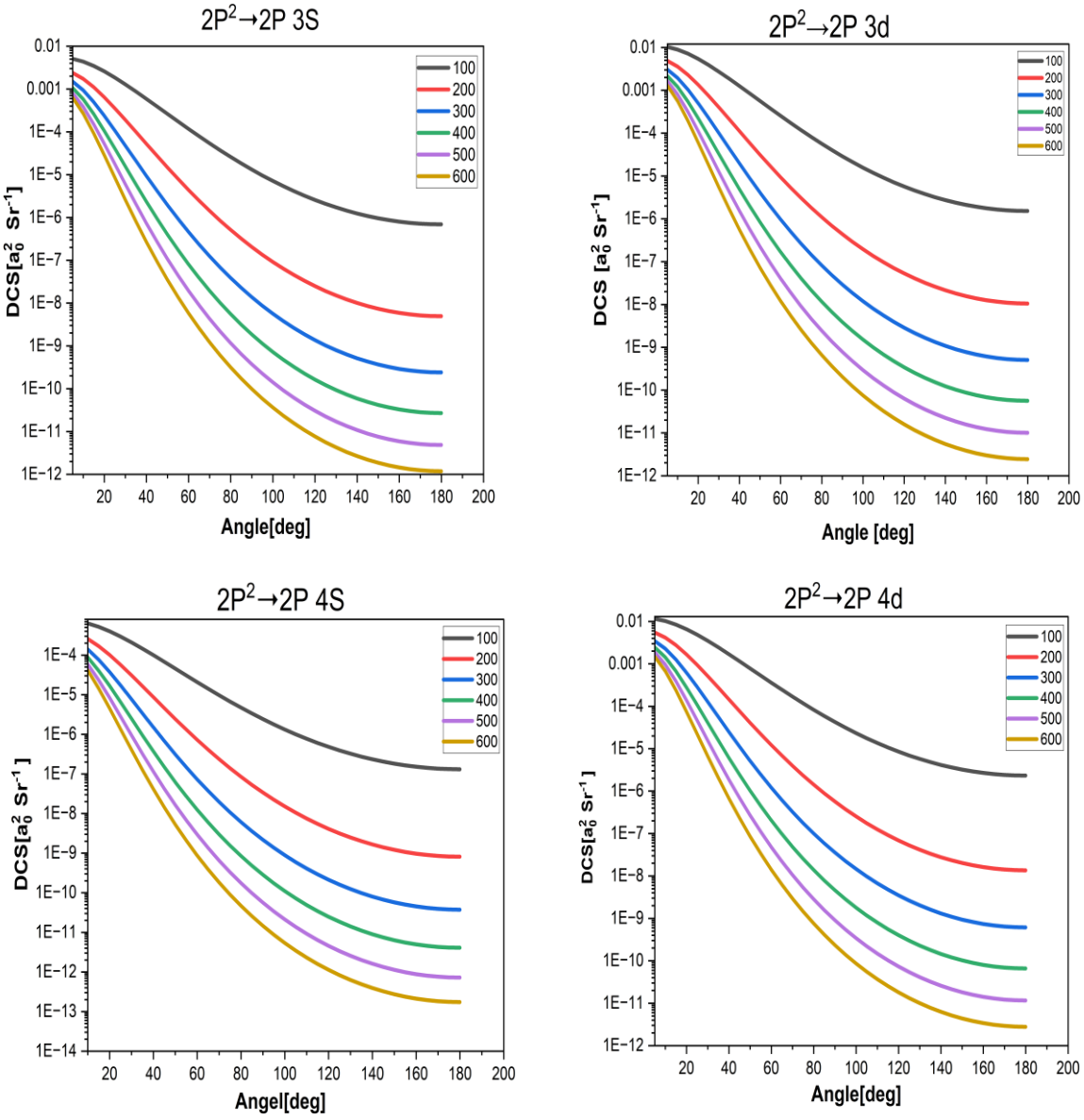

Figure 3: The Differential Excitation Cross Section for Electron Impact with N II for different transitions. The solid lines represent the present work

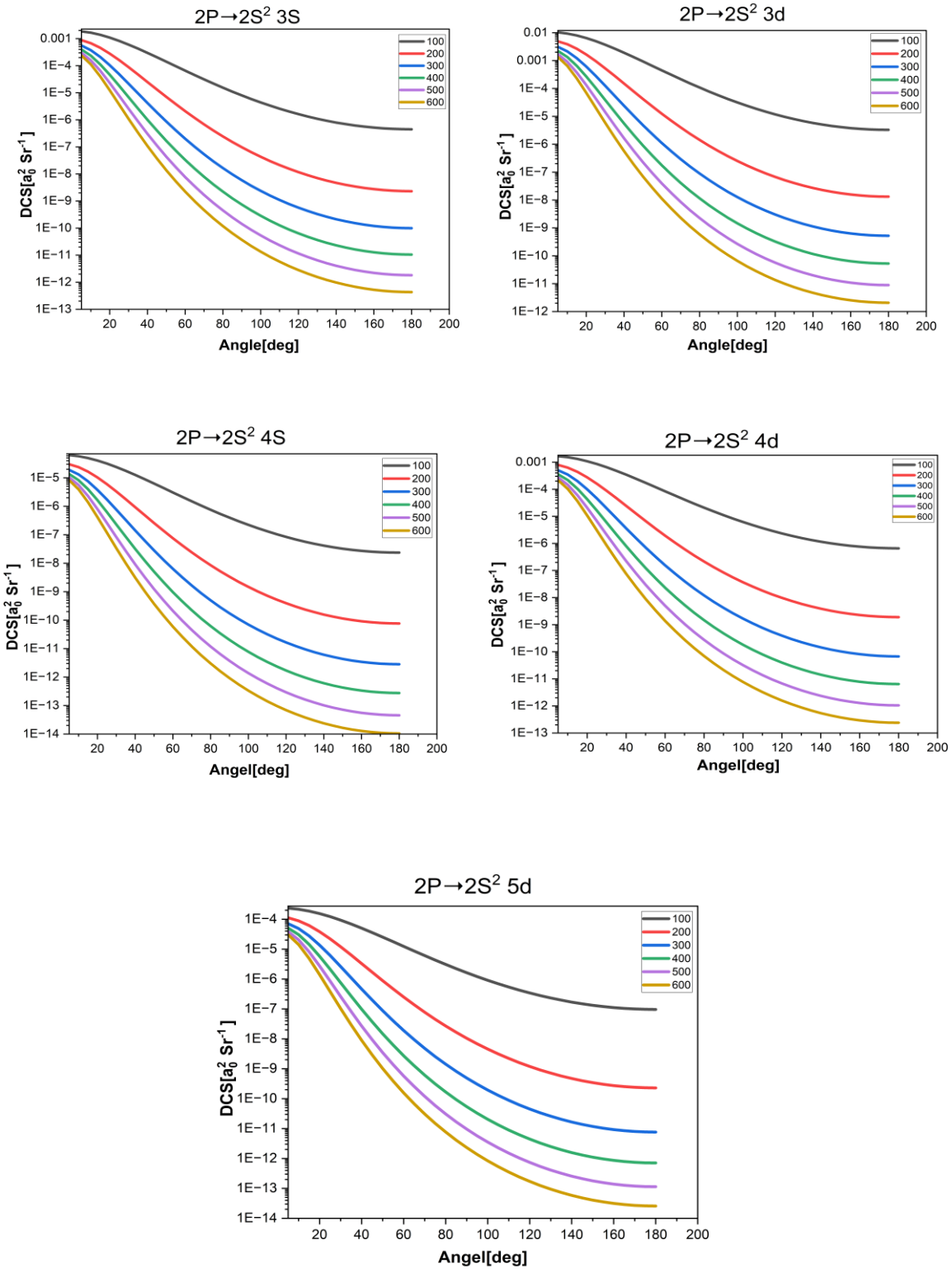

Figure 4: The Differential Excitation Cross Section for Electron Impact with N III for different transitions.the solid line is the present work

In Figure 5, the current work presents the generalized oscillator strength for the excitation of the nitrogen ion (N II) across a set of excitation states. All the calculated transitions have been compared with the theoretical study that utilized the independent particle model in its calculations(Ganas, 1980). In one of the transitions $2P^2 \rightarrow$ 2P 3S Our results demonstrate a substantial similarity to the theoretical predictions, with only a slight difference observed. However, for another transition $2P^2 \rightarrow 2P\ 3d$. The results do not closely align with the theoretical predictions. While another transition $2P^2 \rightarrow 2P\ 4S$, A similar pattern is shown between our results and the theoretical predictions, but a noticeable difference remains. In contrast, for yet another transition $2P^2 \rightarrow 2P$ 4d our results are nearly identical to the theoretical predictions, indicating excellent agreement.

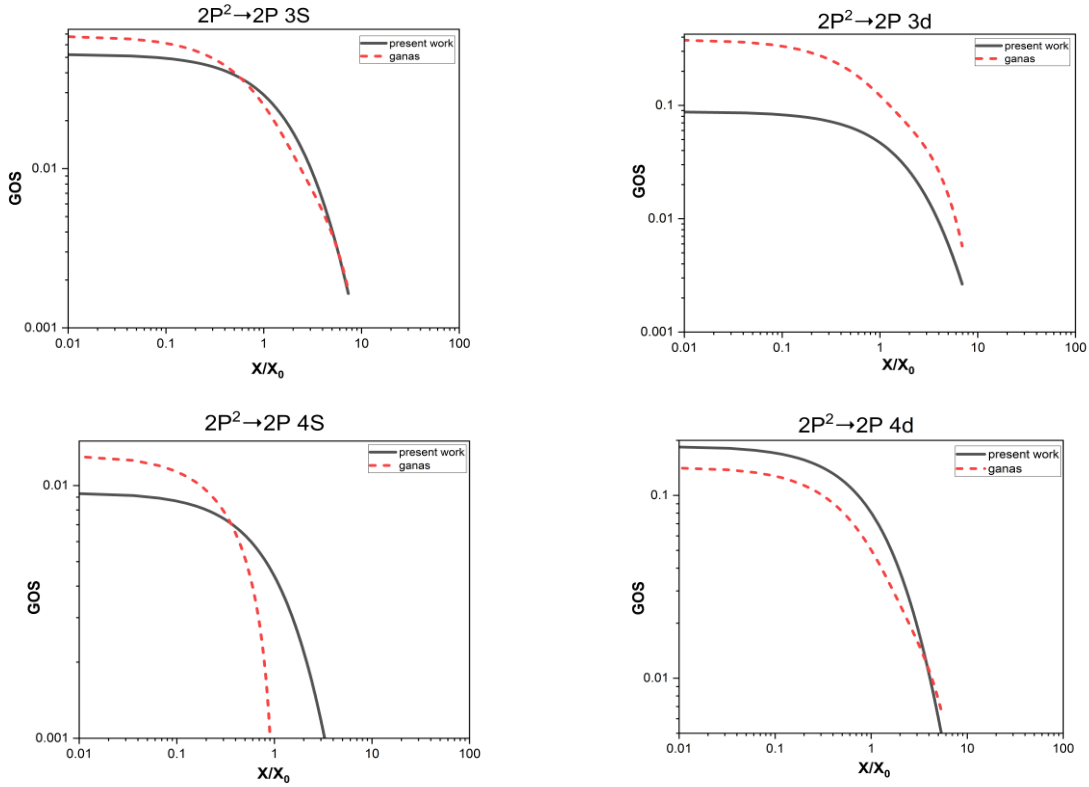

Figure 5: The Generalized Oscillator Strength for Electron Impact with N II for different transitions. The solid lines represent the present work, and the short, dashed line represents the study by(Ganas, 1980)

As with the previous ion, Figure 6 presents the results for the nitrogen ion, displaying the calculations for various excitation transitions. These results have been compared with the theoretical study conducted by(Ganas, 1979), which utilized the independent particle model in its calculations. In the first transition, $2P \rightarrow 2S^2 3S$, we observed a difference and divergence between our results and the theoretical predictions. In another transition, $2P \rightarrow 2S^2$ 3d, and the results demonstrate impressive agreement with the theoretical predictions. The results for a different transition from $2P \rightarrow 2S^2$ 4S are outstanding and nearly identical to the theoretical predictions. In the other transitions,$2P \rightarrow 2S^2$ 4d, although $2P \rightarrow 2S^2$ 5d, there are no issues with the shape of the function between our results and the theoretical predictions; a noticeable difference can be observed in the graph.

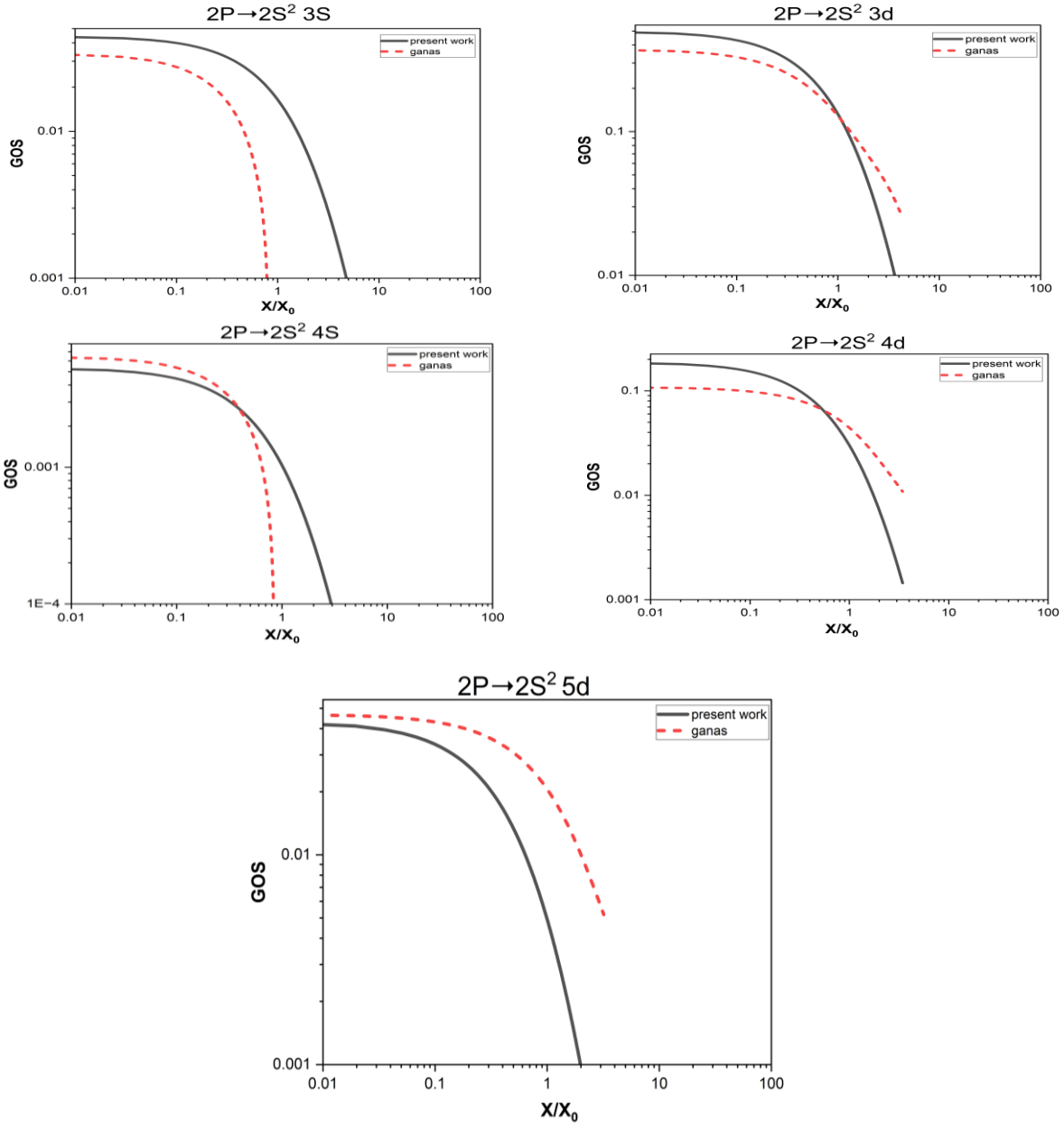

Figure 6: The Generalized Oscillator Strength for Electron Impact with N III for different transitions. The solid lines represent present work, and the short-dashed line represents the results of studies by (Ganas, 1979)

This article calculated the radiation transition probabilities and lifetimes for the states under investigation, which are presented in Tables 3 and 4. Additionally, we computed the oscillator strength.

Table 3: The calculated oscillator strength, transition probability (sec^{-1}), and lifetime (sec) for some allowed states for N II

Transition	Excitation Energy(eV)	Oscillator strength	Transition Probability$\times 10^{7}$	Life Time $\times 10^{-7}$
$2P^2 \rightarrow 2P\ 3S$	18.4562(Wiese et al., 1966)	0.0371	0.1938	5.1599
$2P^2 \rightarrow 2P\ 3d$	19.5193(Wiese et al., 1966)	0.0882	0.3649	2.7427
$2P^2 \rightarrow 2P\ 4S$	22.6323(Wiese et al., 1996)	0.0098	5.2534	0.1903
$2P^2 \rightarrow 2P\ 4d$	24.2745(Wiese et al., 1996)	0.1863	0.0119	84.033

Table 4: The calculated oscillator strength, transition probability (sec^{-1}), and lifetime (sec) for some allowed states for N III

Transition	Excitation Energy(eV)	Oscillator strength	Transition Probability$\times 10^{7}$	Life Time $\times 10^{-7}$
$2P \rightarrow 2S^2 3S$	27.4379(Wiese et al., 1966)	0.0443	0.3627	2.7570
$2P \rightarrow 2S^2 3D$	33.1194(Wiese et al., 1996)	0.4988	0.0594	16.835
$2P \rightarrow 2S^2 4S$	37.3078(Wiese et al., 1996)	0.0053	7.0669	0.1415
$2P \rightarrow 2S^2 4D$	39.2980(Wiese et al., 1996)	0.1879	0.0316	31.645
$2P \rightarrow 2S^2 5D$	42.3744(Wiese et al., 1996)	0.0432	0.7383	1.3544

Conclusions:

In this paper, we present the results for the generalized oscillator strength (GOS), differential cross section (DCS), integral cross section (EXCS), transition probabilities, and lifetimes for the excitation of the nitrogen ions (N II and N III) when colliding with electrons at energies ranging from 1 eV to 1000 eV. The calculations were performed using the Born-Bethe approximation, which has proven effective in addressing the excitation of nitrogen ions by fast electrons. Our calculated results demonstrate good agreement with the theoretical data used for comparison. However, some discrepancies are observed in Figure 4 for the transitions $2P^2 \rightarrow 2P\ 4d$ in the nitrogen ion N II and $2p \rightarrow 2S^2\ 5d$ in the nitrogen ion N III. These discrepancies can be attributed to the low calculated oscillator strength, affecting the computed cross-section values. To our knowledge, no experimental data has been recorded for all the calculations performed.

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