

Velocity Form Calculations of Generalized Oscillator Strengths for $3s \rightarrow (3p, 4p, 5p, 6p)$ Dipole Transitions of Atomic Sodium in Debye Plasma

Louis Gomis*, Clement Diatta, Moustapha Sadibou Tall, Ibrahima Gueye Faye, Rama Gomis, Yande Diouf, Mamadou Coulibaly

Laboratoire de Physique des Plasmas et de Recherches Interdisciplinaires, Departement de Physique, Universite Cheikh Anta Diop, Dakar, Senegal

Email: *lgomis73@yahoo.fr

How to cite this paper: Gomis, L., Diatta, C., Tall, M.S., Faye, I.G., Gomis, R., Diouf, Y. and Coulibaly, M. (2024) Velocity Form Calculations of Generalized Oscillator Strengths for $3s \rightarrow (3p, 4p, 5p, 6p)$ Dipole Transitions of Atomic Sodium in Debye Plasma. *Open Journal of Applied Sciences*, 14, 1512-1529. <https://doi.org/10.4236/ojapps.2024.146101>

Received: May 16, 2024

Accepted: June 21, 2024

Published: June 24, 2024

Copyright © 2024 by author(s) and Scientific Research Publishing Inc.

This work is licensed under the Creative Commons Attribution International License (CC BY 4.0).

<http://creativecommons.org/licenses/by/4.0/>



Open Access

Abstract

In this paper, the generalized oscillator strengths (GOSs) of excitations of atomic sodium from ground state to $2p^63s^0$ ($3p, 4p, 5p, 6p$) states, immersed in Debye plasma, were calculated by using wavefunctions which were obtained numerically from the restricted Hartree-Fock (RHF) equation. This RHF equation employs the local density approach for exchange interactions including plasma Debye screening. Theoretical RHF and random phase approximation with exchange (RPAE) velocity calculations have shown that the GOSs for excitations to $3s^0$ ($3p, 4p, 5p, 6p$) depend on the plasma Debye screening effects, as shown by the reduction in the *GOS* amplitude with decreasing Debye length λ_D . The agreement between the present RPAE V results for the transitions $3s \rightarrow 3s^0$ ($3p, 4p, 5p$) and the length calculations of Martínez-Flores was satisfactory. Correlation effects were found quite to be significant in the vicinity of the maxima of the *GOS* of the $3s \rightarrow 3s^0$ ($4p, 5p, 6p$) excitations by using the RPAE V approach. We note the poor influence of many electron correlations on the *GOS* of ($3s \rightarrow 3p$) transition with the same principal quantum number. Finally, we comment that the RPAE V calculations are useful in investigating electron correlation effects on the transition *GOS* of atomic sodium planted in Debye plasma. The present velocity results also reveal that the $3s \rightarrow 3s^0$ ($5p, 6p$) transition *GOS*s tend to be delocalized due to more significant screening effects at Debye lengths $\lambda_D = 20$ and 30 a.u. for excited subshells 5p and 6p, respectively.

We report here novel results of *GOS* for $3s \rightarrow 3s^0 6p$ transition obtained from different Debye lengths.

Keywords

Plasma Screening Effect, Correlation Effect, Sodium Atomic, Velocity Form *GOS*, Restricted Hatree-Fock, Random Phase Approximation with Exchange

1. Introduction

The present aim of this study is to investigate the fast electron inelastic scattering, which is characterized by the generalized oscillator strength (*GOS*). Introduced by Bethe in atomic physics [1], *GOS* provides information on the valence shell excitations of atoms and molecules. The presence of atomic sodium in the atmosphere and its hydrogenlike electronic structure have inspired numerous theoretical [2] [3] and experimental studies. In several studies on the properties of free atomic sodium [1] [4] [5], the significant role of the interaction between atomic electrons has been demonstrated. Other studies have shown that the properties of confined atomic sodium [2] [3] differ from those of free atomic sodium, depending on the nature of the plasma [2]. For example, from their study of Debye plasma, Yue-Ying Qi *et al.* [6] reported their theoretical results of oscillator strengths and dipole polarizabilities of the $3s$ et $3p$ states of the sodium. In the case of *GOS* for the ground state $2p^6 3s$ of atomic sodium, the theoretical work of Martínez-Flores [7] has been reported in the literature. This work was carried out using wavefunctions obtained with the pseudo-potential model to modify the $3s$ valence state. To incorporate the effects of the plasma environment, Martínez-Flores [7] developed pseudopotential model approach to describe the inner electrons. The calculation uses this pseudo-potential to obtain accurate wavefunctions and the *GOS* by applying the length form formulae. From their theoretical works [2] [3] [6] [7], there have been successful efforts to incorporate the plasma screening effects with the elaboration of the pseudo-potential model approach describing the inner-electrons. However, in the study of atomic sodium collisions in plasma environments this pseudo-potential model approach does not include the inner electron exchange contributions. This investigation stimulated full-electron studies of atomic sodium in Debye-plasma. It is therefore of interest to have theoretical calculations with a two fold purposes in mind. The first was to evaluate the *GOS* using an alternative length form. This alternative form is the velocity formulation of the Bethe approximation which is a simple version of the Born approximation [8]. The second is to add another description to investigate the inner electron exchange contributions to account for the *GOS* of the electronic excitations. To supplement this previous work, we point out the application of another technique for many electron problems. The specification of the proposed method is that it considers the

virtual excitations of electrons from other subshells. This approach differs from common calculations in that we directly obtain the *GOS* without constructing a pair of eigenfunctions from an integral equation that describes the collective multi-electron effects.

The remainder of this paper is organized as follows. In Section 2, we provide a theoretical method for determining the atomic orbital energies of sodium atoms in Debye plasma for various screening lengths. Section 3 describes the velocity formulation of the *GOS* in the restricted Hartree-Fock (RHF) and random phase approximation with exchange (RPAE) approaches. In Section 4, we present our *GOS* computational results obtained in velocity form and compare them with other investigations where possible. Finally, in the last Section, we present our conclusions. Atomic units (a.u.) were used throughout this study unless otherwise indicated.

2. Energy for Sodium in a Debye Plasma

As described elsewhere [9], we can find the electronic energy level of atoms by solving the non-relativistic time-independent Schrödinger equation given by:

$$\left[-\frac{d^2}{2dr^2} + \frac{\ell(\ell+1)}{2r^2} + V_{eff}^{\lambda_D}(r) \right] P_{n\ell}(r) = \varepsilon_{n\ell} P_{n\ell}(r) \quad (1)$$

where $V_{eff}^{\lambda_D}$ is the effective potential including the Debye screening and λ_D is the screening length of a Debye plasma. Here $V_{eff}^{\lambda_D}$ can be expressed as:

$$\begin{aligned} V_{eff}^{\lambda_D}(r) = & -\frac{Z}{r} e^{-\frac{r}{\lambda_D}} + \sum_{n\ell} \frac{N_{n\ell}}{\lambda_D} \frac{1}{\sqrt{r}} K_{1/2}\left(\frac{r}{\lambda_D}\right) \left[\int_0^r |P_{n\ell}(r')|^2 \frac{1}{\sqrt{r'}} I_{1/2}\left(\frac{r'}{\lambda_D}\right) dr' \right] \\ & + \sum_{n\ell} \frac{N_{n\ell}}{\lambda_D} \frac{1}{\sqrt{r}} I_{1/2}\left(\frac{r}{\lambda_D}\right) \left[\int_r^\infty |P_{n\ell}(r')|^2 \frac{1}{\sqrt{r'}} K_{1/2}\left(\frac{r'}{\lambda_D}\right) dr' \right] \\ & - 6 \left[\frac{3}{32\pi^2} \sum_{n\ell} \frac{N_{n\ell} [P_{n\ell}(r)]^2}{r^2} \right]^{1/3} \times F(\theta) \end{aligned} \quad (2)$$

If $r < r_0$,

and

$$V_{eff}^{\lambda_D}(r) = \frac{2(Z - N + 1)}{r} \quad (3)$$

if $r \geq r_0$.

Here r_0 is the value of r when Equations (2) and (3) are equated. In the above equations and in the following, we use the notation that Z , $N_{n\ell}$ and N are respectively the atomic number, the occupation number for orbital $n\ell$ and the number of atomic electrons more generally equal to $\sum_{n\ell} N_{n\ell}$. Note that $F(\theta)$ in Equation (2) is the screening function. This screening function is a correction factor which reads [9] [10] [11].

$$F(\theta) = 1 - \frac{\theta^2}{6} - \frac{4}{3}\theta \tan^{-1}\left(\frac{2}{\theta}\right) + \frac{\theta^2}{2}\left(1 + \frac{\theta^2}{12}\right) \ln\left|1 + \frac{2}{\theta^2}\right| \quad (4)$$

where $\theta = \frac{k_s}{k_F} = \frac{1}{\lambda_D k_F}$ is defined as the ratio of the Debye screening parameter $k_s \equiv \frac{1}{\lambda_D}$ to the Fermi momentum k_F . As can be expected from its formulae there is no screening for $k_s = 0$ (i.e., $\lambda_D \rightarrow \infty$). It can be seen in Equation (2), $I_{1/2}(r)$ and $K_{1/2}(r)$ which are obtained using the modified Bessel functions of the first kind $I_{k+1/2}(r)$ and the second kind $K_{k+1/2}(r)$, respectively for the case of $k=0$. In this study, we develop a procedure to perform Equation (1) obtained by considering Debye screening in the restricted Hartree-Fock approach. In this procedure, Equation (1) is converted into an eigenvalue equation, where the different eigenvalues are the orbital energies. The eigenvalue problem can be solved by using a computation technique based on finite difference approximations to numerically calculate the *orbital energies* and *radial wavefunctions* with good efficiency. Calculations of the atomic sodium structure in Debye plasma were numerically performed using MATLAB software. We calculated the atomic sodium *orbital energy* for the ground state 3s and excited states 3p, 4p, 5p and 6p for a number of Debye lengths.

In **Table 1** and **Table 2**, we compare the present *energy levels* for 3s, 3p, 4p, 5p and 6p states for atomic sodium in Debye plasmas of different screening lengths with the theoretical data from references [6] [7] [9]. The theoretical data of Bunjac *et al.* [9] for the free case and the results from Qi *et al.* [6] for Debye Screening are in good agreement with those found in this work. This agreement between the results from references [6] [9] and our findings is greater than 3.5%. From **Table 1** and **Table 2**, the power values of alphabet letter **a** and those in power of alphabet letter **b** are the theoretical results of Martínez-Flores [7] for atomic.

Table 1. Energy of 3s and 3p orbitals for atomic sodium in plasmas of different screening lengths.

λ_D	ε_{3s} (a u)				ε_{3p} (a u)				
	PT	[6]	[7]	PT	[6]	[7]	[9]		
∞	-0.18269	-0.18886	-0.18884 ^a	----	-0.11020	-0.11152	-0.11152 ^a	----	-0.11241
100	-0.17350	-----	-0.17810 ^a	-0.17790 ^b	-0.10099	-----	-0.10146 ^a	-0.10119 ^b	----
50	-0.16652	-0.16780	-0.16778 ^a	-0.16701 ^b	-0.09231	-0.09196	-0.09196 ^a	-0.09093 ^b	----
33	-0.15791	-0.15758	-----	-----	-0.08390	-0.08273	----	-----	----
30	-0.15545	-----	-0.15464 ^a	-0.15263 ^b	-0.08153	-----	-0.08012 ^a	-0.07748 ^b	----
20	-0.14868	-----	-0.13918 ^a	-0.13498 ^b	-0.06919	-----	-0.06658 ^a	-0.06124 ^b	----

Table 2. Energy of 4p, 5p and 6p orbitals for atomic sodium in plasmas of different screening lengths.

λ_D	ε_{4p} (a.u)					ε_{5p} (a.u)					ε_{6p} (a.u)				
	PT	[6]	[7]	[9]	PT	[6]	[7]	[9]	PT	[6]	[7]	[9]	PT	[6]	[9]
∞	-0.05124	-0.05102	-0.05102 ^a	-0.05130	-0.02948	-0.0292	-0.02924 ^a	-0.02937	-0.01968	-0.01894					
100	-0.04236	-----	-0.04157 ^a	-----	-0.02067	-----	-0.02033 ^a	-----	-0.01107	-----					
50	-0.03463	-0.03333	-0.03332 ^a	-----	-0.01381	-0.01341	-0.01340 ^a	-----	-0.00764	-0.00511					
33	-0.02771	-0.02596	-----	-----	-0.00842	-0.00799	-----	-----	-0.00437	-----					
30	-0.02587	-----	-0.02400 ^a	-----	-0.00712	-----	-0.00669 ^a	-----	-0.00370	-----					
20	-0.02157	-----	-0.01473 ^a	-----	-0.01543	-----	-0.00169 ^a	-----	-0.01399	-----					

Sodium, respectively in the presence of Debye plasma and strong plasma described by the exponential-cosine-screened coulomb potential (ECSC). We note that the agreement for the *energy orbital* is generally good for some values of the *Debye length*, except for $\lambda_D = 20$. In this case $\lambda_D = 20$, and we obtained the present computed *orbital energy* $\varepsilon_{3p} = -0.01543$, in disagreement with $\varepsilon_{3p} = 0.00169$ which is the theoretical result from Martínez-Flores [7]. This discrepancy may be explained by the fact that the present *orbital energy* of 5p is overestimated when the *Debye length* λ_D approaches a critical screening length. We also note the abrupt change between the two values of E_{6p} for $\lambda_D = 30$ and $\lambda_D = 20$ which can be attributed to the same reason mentioned above.

3. Velocity Formulation of GOS

3.1. In RHF Method

With the Bethe-Born Theory [10], the *GOS* accounts for the probability of excitation from the initial state with the wavefunction $|\psi_o\rangle$ to a final excited state described by the wavefunction $|\psi_f\rangle$ obtained by means of the alternative length form, defined as [11]:

$$F_{of}(\omega, q) = \frac{2\omega}{q^2} \left| \sum_{j=1}^N \int \psi_f(\vec{r}_1 \vec{r}_2 \cdots \vec{r}_N) \times \left(\frac{1}{2\omega} \left[\exp(i\vec{q} \cdot \vec{r}_j) (q\nabla_j) - (q\bar{\nabla}_j) \exp(i\vec{q} \cdot \vec{r}_j) \right] \right) \times \psi_o(\vec{r}_1 \vec{r}_2 \cdots \vec{r}_N) d\vec{r}_j \right|^2 \quad (5)$$

where \vec{r}_j is the vector position of electron j , q is the transferred momentum, ω is the energy transferred. In this equation, the upper arrow in the Nabla operator indicates that it operates on the function standing to the left.

The atomic state wavefunctions $\psi_{of}(\vec{r}_1 \vec{r}_2 \cdots \vec{r}_N)$ are Slater determinants built from spin orbitals. The spin orbitals are one-electron wave functions taking both their positions and spin angular momentums of atomic electrons which obey Pauli's exclusion principle and Hund's rule. The Slater determinant satisfies the anti-symmetry property because it can be expanded as a linear combination of one-electron functions. In the integration procedure of Equation (5), we have the normalization and orthogonality conditions that allow us to write the expression of $F_{of}(\omega, q)$ as the sum of the *GOS* terms associated only with the transition of one electron from the state denoted by s to the state denoted by t .

$$F_{of}(\omega, q) = \sum_{st} f_{st}(\omega, q) \quad (6)$$

where $f_{st}(\omega, q)$ is the *GOS* term.

We consider that one electron of the initial state s is promoted to an excited state t under the assumption that the other electrons remain in the Debye plasma environment without leaving their initial subshells. In this case the *GOS* term is given by:

$$f_{st}(\omega, q) = \frac{2\omega}{q^2} \left| \sum_{j=1}^N \int \phi_t(\vec{r}) \left(\frac{1}{2\omega} \left[\exp(i\vec{q} \cdot \vec{r})(q\nabla) - (q\nabla)\exp(i\vec{q} \cdot \vec{r}) \right] \right) \phi_s(\vec{r}) d\vec{r} \right|^2 \quad (7)$$

where $\phi_s(\vec{r})$ and $\phi_t(\vec{r})$ are the one-electron RHF wavefunctions of the initial and final states for each electron, respectively, when the energy conservation law $\omega = \varepsilon_t - \varepsilon_s$ is satisfied.

By inserting the operator $\exp(i\vec{q} \cdot \vec{r})$ into the spherical wave expansion form and $\phi_{s(t)}(\vec{r})$ as a product of the radial, angular and spin functions, it allows the nabla operator in Equation (7) by using its spherical coordinate system to operate on the radial and spherical harmonic functions. Then, by integrating the angular and spin parts of the *GOS* term, we obtain that *GOS* $f_{st}(\omega, q)$ can be expanded in terms of the total angular momentum ℓ in the form [12] [13]:

$$f_{st}(\omega, q) = \sum_{\ell=|\ell_t-\ell_s|}^{|\ell_t+\ell_s|} f_{st}^{\ell}(\omega, q) \quad (8)$$

In Equation (8), f_{st}^{ℓ} is the ℓ multipole *GOS*, we have the total angular momentum ℓ of the electron-hole pair taking values: $|\ell_t - \ell_s|$; $|\ell_t - \ell_s| + 2$; \dots ; $|\ell_t + \ell_s|$.

In the velocity formulation, the multipole *GOS* f_{st}^{ℓ} is defined as follow:

$$f_{st}^{\ell}(\omega, q) = \frac{2\omega N_s (2\ell + 1)}{q^2 (2\ell_s + 1)} \left| \frac{q \cdot \begin{pmatrix} \ell_t & \ell & \ell_s \\ 0 & 0 & 0 \end{pmatrix}}{2\omega (2\ell + 1)} \sqrt{(2\ell_t + 1)(2\ell_s + 1)} \right. \\ \times \left\{ \int_0^{\infty} P_{n_s, \ell_s}(r) \frac{j_{\ell-1}(q \cdot r) - j_{\ell+1}(q \cdot r)}{r} P_{n_t, \ell_t}(r) [\ell_t(\ell_t + 1) - \ell_s(\ell_s + 1)] dr \right. \\ \left. + \int_0^{\infty} [(\ell + 1)j_{\ell+1}(q \cdot r) - \ell j_{\ell-1}(q \cdot r)] \left(P_{n_t, \ell_t}(r) \frac{dP_{n_s, \ell_s}(r)}{dr} - P_{n_s, \ell_s}(r) \frac{dP_{n_t, \ell_t}(r)}{dr} \right) dr \right\} \Bigg|^2 \quad (9)$$

In this Equation (9), $P_{n_s, \ell_s}(r)$ and $P_{n_t, \ell_t}(r)$ are also normalized radial functions of initial and final RHF wavefunctions, respectively and $j_{\ell}(q \cdot r)$ is the spherical Bessel function of the first kind. Equation (9) is used as an approximation to include only one electron of the screened atomic sodium that participates directly in the collision process. This approach, while describing the fast charged particle collisions with atomic sodium in the first-Born approximation, does not account for the exchange interaction of other atomic electrons. The impact of the incident charged particle on all the atomic electrons to which its energy is transferred, can be considered in the framework of the RPAE.

3.2. In RPAE Approach

To introduce other means of electron excitation with the creation of an electron-hole pair in the calculation of the inelastic scattering *GOS* of a polyelectronic atom, one may use the RPAE description according to [13]. RPAE is based on a residual interaction because an electron excited from an atom by scattering can excite another atomic electron. The RPAE approximation enables us to treat the virtual transitions in this frame of a many-electron picture. The

following considerations make it possible to write an equation for the *matrix transition* as [11] [13] [14]:

$$\begin{aligned} & \langle \phi_t(r) | V^{RPAE}(\omega, q) | \phi_s(r) \rangle \\ &= \langle \phi_t(r) | \left[\frac{1}{2\omega} \left[\exp(i\vec{q} \cdot \vec{r}_j) (q \nabla_j) - (q \bar{\nabla}_j) \exp(i\vec{q} \cdot \vec{r}_j) \right] \right] | \phi_s(r) \rangle \\ &+ \left(\sum_{p \leq F, r \geq F} - \sum_{r \leq F, p \geq F} \right) \frac{\langle \phi_r(r) | V^{RPAE}(\omega, q) | \phi_p(r) \rangle}{\omega - \varepsilon_r + \varepsilon_p + i\alpha(1 - 2\eta_r)} \\ &\times \langle \phi_p(r) \phi_t(r) | U | \phi_s(r) \phi_t(r) \rangle \end{aligned} \quad (10)$$

Here $V^{RPAE}(\omega, q)$ is the multipole nonlocal operator in the velocity formulation that describes multi-electron correlations. $\langle \phi_p(r) \phi_t(r) | U | \phi_s(r) \phi_t(r) \rangle$ represents the combination of the direct and exchange matrix elements of the electron-electron interaction ϕ_r (ϕ_p) is the final (initial) virtual excitation state with their corresponding final (initial) *orbital energy* ε_r (ε_p). F is the Fermi level of the sodium atom and the Fermi step function β_k appears as follows $\eta_r = 1(0)$ for occupied (vacant) states. The complex number $i\alpha$ in the denominator of Equation (10), with the imaginary part $\alpha \rightarrow 0^+$ just gives us the direction of tracing the pole in integration.

Numerical study of the accuracy and efficiency of discrete excitations is very difficult because some terms of the denominators in Equation (10) become zero at $\omega = \varepsilon_r - \varepsilon_p$ in the calculations. The procedure described in detail in [15] to eliminate the divergent term from the sum in Equation (10) was used to calculate the *GOS* in the lowest order with respect to U using the following velocity expression:

$$f_{st}^{RPAE}(\omega, q) = \frac{|V_{st}^{RPAE}(\omega, q)|^2}{1 + \sum_{(st) \neq (rp)} \frac{|U_{strp}|^2}{(\omega - \varepsilon_r + \varepsilon_p)^2}} \quad (11)$$

where, we consider $V_{st}^{RPAE}(\omega, q)$ as a solution to Equation (10) with terms without the non vanishing denominator. Here $U_{strp} \equiv \langle \phi_p(r) \phi_t(r) | U | \phi_s(r) \phi_t(r) \rangle$ denotes the combination of direct and exchange matrix elements of the interaction electron-electron.

4. Results of *GOS* Calculations in Velocity Form for Na Atom

From Equations (9) and (11), we computed the *GOS* of the atomic sodium $3s \rightarrow (3p, 4p, 5p, 6p)$ dipole transitions in the present velocity calculations. In order to illustrate the competition between shell electron interaction and plasma screening effect, our results are presented below and compared with those of other authors.

4.1. *GOS* of 3s to 3p Excitation

The behavior of the RHF and RPAE *GOS* for the $3s \rightarrow 3p$ dipole transition of

atomic sodium calculated in the present work for various Debye lengths ($\lambda_D = \infty, 100, 30, 20$), is depicted in **Figure 1**. Where they are compared with the results of other authors obtained in their experimental [16] [17] and theoretical studies [1] [7]. In **Figure 1(a)**, we quote the velocity results of the dipole $3s \rightarrow 3p$ transition for the Debye length $\lambda_D = \infty$. The curves of our results and those obtained by Martínez-Flores [7] for $\lambda_D = \infty$ have the same shape as those of the experimental [16] [17] and theoretical [1] results for the free case. In all cases in **Figure 1**, we also note that the *GOS* converges to zero for all Debye lengths λ_D when going from a larger momentum transfer q . This convergence is due to the fact that atomic electrons cannot receive momentum transfer greater than a limit determined by the uncertainty principle without recoiling out of the atom. In **Figure 1(a)**, there is agreement with the results above the momentum transfer $q = 0.2$ a.u. A discrepancy was noted between our calculated data and the results of Martínez-Flores [7] and Han *et al.* [1] for transferred momentum $q \leq 0.2$ a.u. This discrepancy does not exceed 6.20% and 9.40% for RHF-V and RPAE-V, respectively. This difference between may be attributed to the nature of the difference wavefunctions used in the work. The *GOS* from RHF-V shows a slight difference from that of RPAE-V at $q \leq 0.2$ a.u. The effects of electronic correlations on the *GOS* $3s \rightarrow 3p$ dipole transition, in this region are greatly appreciated. Their contribution to the present RPAE-V.

Framework is approximately 3.2%. In **Figure 1(b)** and **Figure 1(c)**, we find agreement between the RHF-V and RPAE-V calculations in the transferred momentum interval $[0.2, 1]$ while a small disagreement between them is seen in the interval $[0, 0.2]$ where we note that the RHF-V curves lie above the RPAE-V curves. The results of our two calculations agree well in the q region of $0 - 1$ a.u. in **Figure 1(d)**. This situation can be explained by the fact that the correlation effects have less influence than the plasma Debye screening effects on the *GOS* when the Debye lengths decrease.

To observe the Debye screening effect on the *GOS* of the atomic sodium excitation from the ground state to $3p$, the RHF-V and RPAE-V *GOS* results were obtained for Debye lengths $\lambda_D = \infty, 100, 30$ and 20 a.u. are shown in **Figure 2**. **Figure 2(a)** shows the RHF-V results for these various Debye lengths while the RPAE-V ones are found in **Figure 2(b)**. As can be seen, the absolute values of this *GOS* for $\lambda_D = 20$ are the smallest to the transferred momentum $q \leq 0.5$ a.u. Above this value of $q = 0.5$ a.u., all *GOS* curves are so close together. However, this is not the case when $q < 0.5$ a.u. Note that the amplitude of the *GOS* for the dipole transition diminishes as the Debye length λ_D decreases. In this case where q tends towards zero, the RPAE-V *GOS* values are 1.066, 1.017 and 0.9600 for $\lambda_D = \infty$, $\lambda_D = 100, 30$ and $\lambda_D = 20$ respectively. The present value 1.066 of the dipole oscillator strength is in the accordance with the theoretical value 1.05 listed in reference [18] because their agreement does not exceed 1.53%. From **Figure 2(a)**, a similar situation can be observed for the results obtained from the RHF-V calculations. This indicates that the Debye

screening effects play a very important role in the modification of the *GOS*'s value at low q for the $3s \rightarrow 3p$ atomic sodium transition.

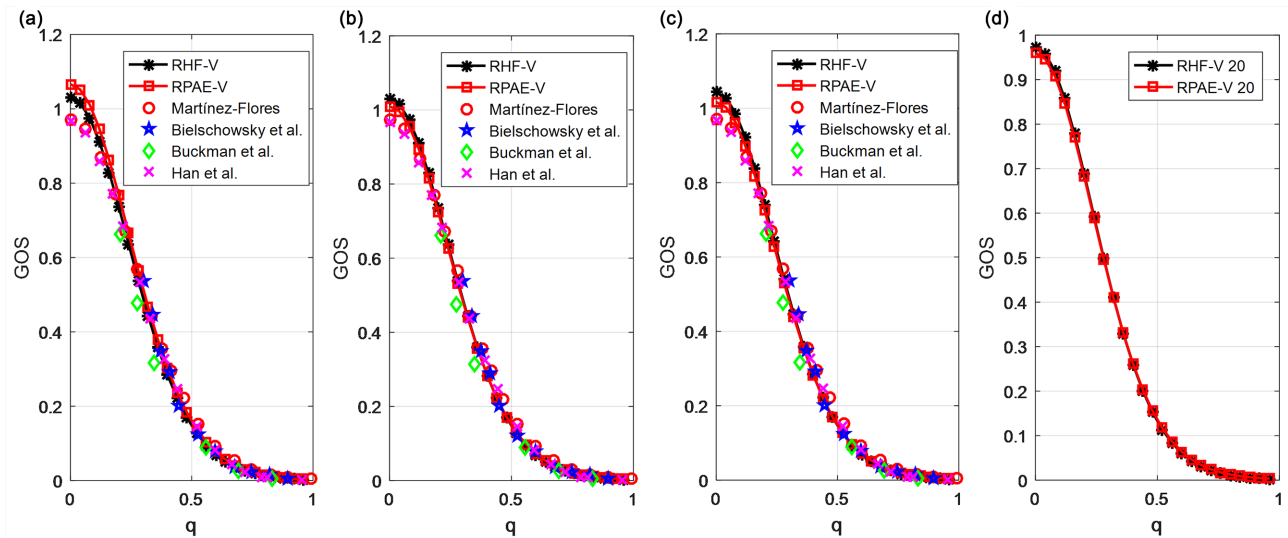


Figure 1. Generalized oscillator strength as a function of the transferred momentum q for sodium atom $3s$ to $3p$ transition. In (a) for $\lambda_D = 10^{10}$ (infty), the RPAE (red solid square line) and RHF (black solid asterisk line) results in comparison with the experimentally data by Bielschowsky *et al.* [16] (blue star symbol) and Buckman *et al.* [17] (green diamond symbol), and with those theoretically values of Martínez-Flores [7] (red circle symbols) and Han *et al.* [1] (magenta cross symbols). In (b), for a screening length $\lambda_D = 100$, in (c) for a screening length $\lambda_D = 30$, in (d) screening length $\lambda_D = 20$.

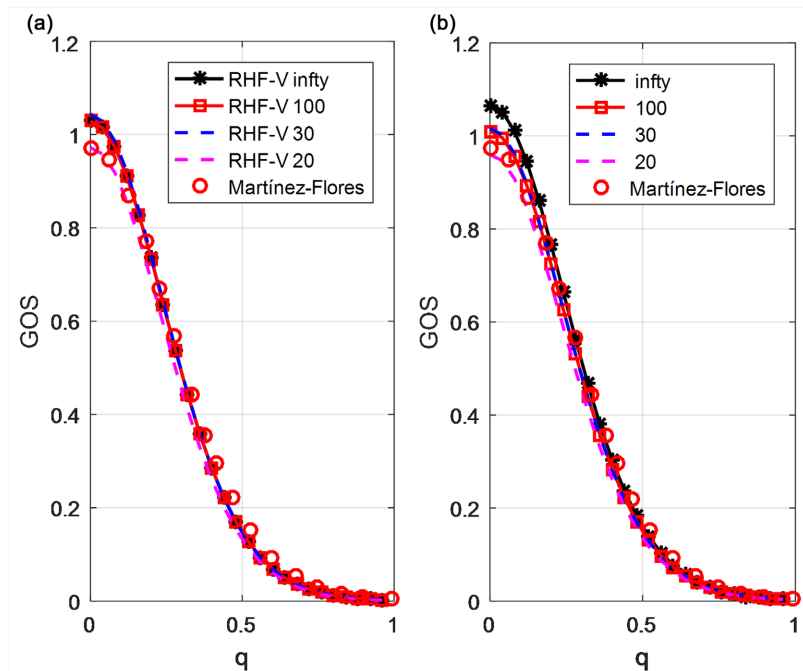


Figure 2. Velocity generalized oscillator strength as a function of the transferred momentum q for atomic sodium $3s$ to $3p$ transition. The velocity form calculations were performed for the values of the screening parameter $\lambda_D = 20, 30, 100$ and ∞ . The curves in (a) are our RHF-V results while those in (b) represented our RPAE-V theoretical data.

4.2. GOS of Excitation 3s to 4p

Once, the *GOS* of the atomic sodium dipole transition $3s \rightarrow 3p$ was calculated, we determined the *GOS* for dipole transition of the excitation $3s$ to $4p$. Our computed data are shown for the $3s \rightarrow 4p$ atomic sodium in **Figure 3**. Let us note that **Figures 3(a)-(d)** show respectively the curves of the *GOS* for $\lambda_D = \infty, 100, 30$ and 20 . Some of the data calculated in the present study are compared with those obtained in the length formulation by Martínez-Flores [7] in **Figures 3(a)-(c)**. We remark that the same shape of the *GOS* is observed in these figures and a decrease in their magnitude until reaching zero around the momentum transfer $q = 1.5$ a.u. The findings of *GOS* are in good agreement with the length results of Martínez-Flores [7], except in the q region of $0 - 0.4206$ a.u, as shown in **Figure 3(c)**. For $q \leq 0.4206$, the velocity *GOS* values obtained in this case $\lambda_D = 30$, were less important than those found theoretically by Martínez-Flores [7]. The difference between them does not exceed 6.92%. This discrepancy may be attributable to the variation in the wavefunctions for small atomic electron radius obtained in the two different calculations. Finally, **Figures 3(a)-(d)** also show that the RPAE-V curves lie slightly.

Above the curves of RHF-V particularly around the region of the maxima. As shown in **Figure 3**, the correlation effects do not have much influence on the *GOS* for the $3s \rightarrow 4p$ dipole transition. Their contribution does not exceed 3%. **Figure 4** presents the *GOS* of the atomic sodium $3s \rightarrow 4p$ dipole transition for Debye lengths values $\lambda_D = \infty, 100, 30$ and 20 . The results of our RHF-V calculations are compared in **Figure 4(a)**, while the comparison between the present RPAE-V *GOS* for different values of λ_D are also shown in **Figure 4(b)**. As in RHF-V and RPAE-V, the calculations give almost the same amplitude of the *GOS* of the $3s \rightarrow 4p$ dipole transition for the values of $\lambda_D = \infty$ and 100 .

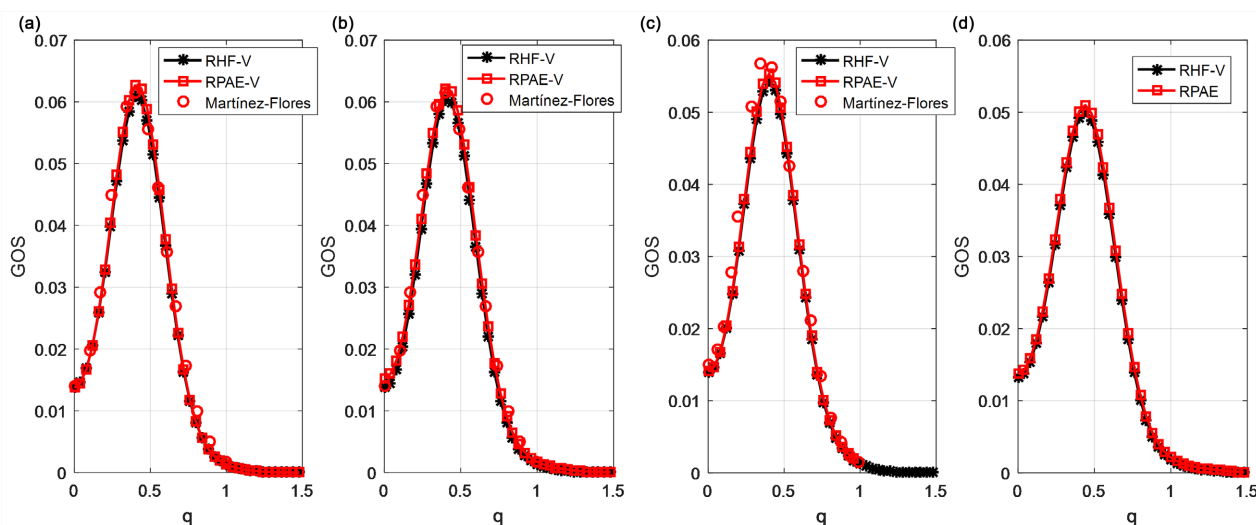


Figure 3. Generalized oscillator strength as a function of the momentum transfer q for sodium atom $3s$ to $4p$ transition. In (a), (b) and (c) Comparison of the *GOS* for the dipole transition theoretically calculated in length formulation by Martínez-Flores [7] with that theoretically calculated in present work by using RHF-V and RPAE-V methods. In frame (d) magenta dashed and blue solid curves represent the RHF-V and RPAE-V data, respectively for the screening parameter $\lambda_D = 20$.

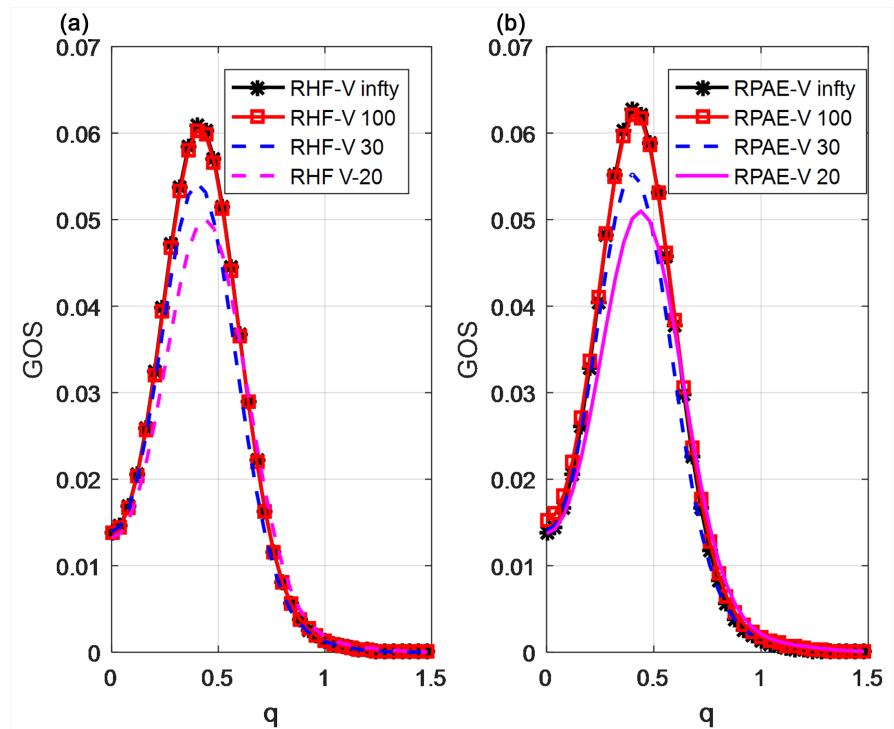


Figure 4. Velocity generalized oscillator strength as a function of the transferred momentum q for atomic sodium 3s to 4p transition. The velocity form calculations were performed for the values of the screening parameter $\lambda_d = 20, 30, 100$ and ∞ . The curves in (a) are our RHF-V results while those in (b) represented our RPAE-V theoretical data.

Note also that the amplitude of the GOS for the dipole transition decreases with the decrease in Debye length $\lambda_d = 100, 30, 20$ and the maxima shift for the last value of this selected set of the screening length. In the RPAE-V approximation, the maximum GOS obtained for the Debye length $\lambda_d = 100$ is 1.1335, which is larger than the corresponding value for the Debye length $\lambda_d = 30$ while this ratio becomes 1.1209 in the RHF-V method. We found that the amplitude of the GOS for Debye length value $\lambda_d = 20$ was slightly less than that calculated for the value of $\lambda_d = 30$. The ratio calculated in this case is approximately 0.9222 in the RPAE-V approach, whereas in the RHF-V method, we obtained 0.9229. The GOS of atomic sodium planted in plasma, to absorb energy from the transferred momentum to its electrons can be strongly affected by the increase in strong plasma interactions. We also note the accordance between our theoretical dipole oscillator value and the theoretical ones listed in references [6] [7].

4.3. GOS of Excitation 3s to 5p

In Section 4.2, we present the GOS of our two velocity calculations for the atomic sodium dipole excitation to 5p in **Figure 5**, along with the length form results of Martínez-Flores [7]. It can be observe from **Figure 5(c)** that the RHF-V and RPAE-V GOS values are smaller than those found in the theoretical work of

Martínez-Flores [7] when $q < 0.5055$ a.u. For the dipole transition $3s \rightarrow 5p$ of atomic sodium in the Debye plasma environment, the difference between them in **Figure 5(c)** does not exceed 10.25% in this region of $q \leq 0.5055$ a.u. This difference can be explained by the different radial overlap of the wavefunctions in the calculated *GOS*. Above this value of $q = 0.5055$ a.u., it can be seen from **Figure 5(c)** that there is.

Agreement between the calculated data in our two velocity calculations and the length form existing theoretical values of Martínez-Flores [7] are good. We find agreement between the present RPAE-V calculations and the length form calculations performed earlier in the work of Martínez-Flores [7] in **Figure 5(a)** and **Figure 5(b)** which correspond to the cases with screening lengths $\lambda_D = \infty$ and $\lambda_D = 100$. There is also an obvious difference in absolute values between the RPAE-V *GOS* and our theoretical RHF-V values around their maxima, as seen in **Figure 5(a)** and **Figure 5(b)**, which depict the results of the transition $3s \rightarrow 5p$ for the Debye lengths $\lambda_D = \infty$ and 100. The electronic-correlations contribute respectively 5.55% and 5.99% to the ∞ and 100 values, respectively. They are unimportant when the Debye length takes values of 30 and 20 because the situation is reversed, as observed in **Figure 5(c)** and **Figure 5(d)**. The effect of the correlations on the *GOS* for dipole transition is not pronounced for high plasma screening. The reason reported above can explain that why the present RPAE-V slightly underestimates the results of our RHF-V. This phenomenon may also be explained by the fact that the terms chosen to be neglected in the velocity matrix element transition become important as λ_D decreases. In **Figure 6**, we plot the dipole transition *GOS* as a function of the momentum transfers for Debye lengths $\lambda_D = \infty, 100, 30$ and 20. The curves in **Figure 6(a)** represent the RHF-V *GOS*, whereas those obtained using the RPAE-V approach are shown in **Figure 6(b)**. For both **Figure 6(a)** and **Figure 6(b)**, we observe a decrease in the $3s \rightarrow 5p$ transition *GOS* amplitude with decreasing Debye length λ_D and a shift of the maxima positions towards greater momentum transfer in the case of $\lambda_D = 20$. For both the RHF-V and RPAE-V calculations, the ratio of the *GOS* magnitude obtained with $\lambda_D = \infty$ and the maximum *GOS* for $\lambda_D = 100$ is less than 1.08. In addition, for the considered Debye lengths $\lambda_D = 100$ and $\lambda_D = 30$ this ratio does not exceed 1.41 while it increases to almost 3 for values of 30 and 20 of Debye length λ_D . Therefore, we conclude that the screening effect strongly affects the *GOS* of the dipole transition when the plasma Debye length λ_D approaches the critical plasma screening length value, which is given in reference [6] for each sub-shell of sodium atoms confined in the plasma environment. The free value ($\lambda_D \rightarrow \infty$) of the *GOS* transition $3s \rightarrow 5p$ reaches 0.002115 a.u. and 0.002158 a.u. in the RHF-V and RPAE-V calculations respectively. We find agreement between these values of the present theoretical calculations and the dipole oscillator strength with values of 0.00216 listed in reference [6] [7] and 0.00221 measured by Wiese *et al.* [19].

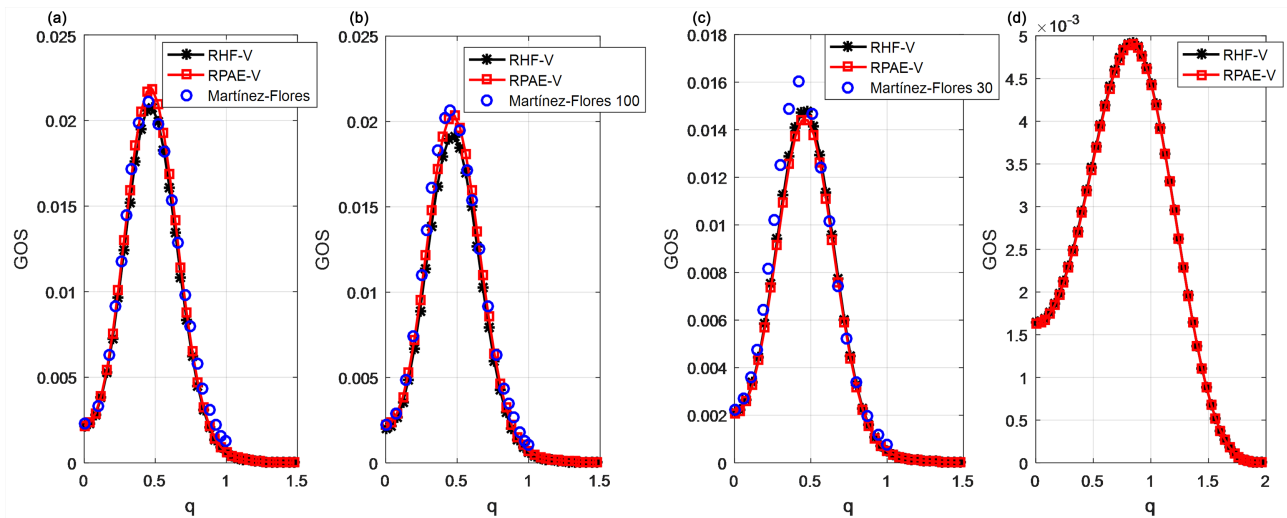


Figure 5. Generalized oscillator strength as a function of the transferred momentum q for sodium atom 3s to 5p transition. In (a), (b) and (c) Comparison of the GOS for theoretically calculated in length formulation by Martínez-Flores [7] with that theoretically calculated in present work by using RHF-V and RPAE-V methods. In frame (d) black solid and red dashed curves represent the RHF-V and RPAE-V data, respectively for the screening parameter $\lambda_d = 20$.

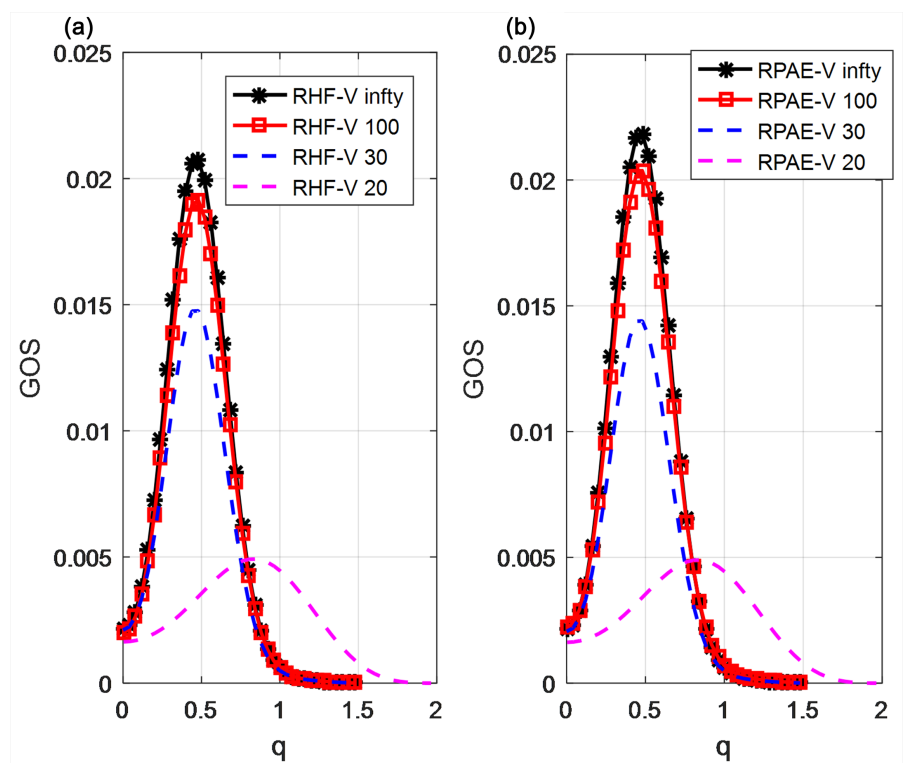


Figure 6. Velocity GOS as a function of the transferred momentum q for atomic sodium 3s to 5p transition. The velocity form calculations were performed for the values of the screening parameter $\lambda_d = 20, 30, 100$ and ∞ . The curves in (a) are our RHF-V results while those in (b) represented our RPAE-V theoretical data.

4.4. GOS of Excitation 3s to 6p

In **Figure 7**, we present the fast charge particle impact excitation of the atomic

sodium transition GOS as a function of the momentum transfer and Debye length. The GOS results are shown in **Figures 7(a)-(c)** for values of $\lambda_D = \infty, 100$ and 30, respectively. Here, we cannot now turn to the results of the $3s \rightarrow 6p$ transition GOS of the sodium atom confined by plasma for $\lambda_D = 20$ because this value is smaller than the critical λ_D value 23.380 listed in **Table 1** of [6]. It can be seen that all the GOS curves have a similar profiles. They also tend towards zero as q increases which is due to the variation of the radial wave functions for a high atomic electron radius.

We note that the correlation effects also have a poor influence on the GOS of the excitation to 6p sub-shell of sodium atoms confined by the Debye plasma environment, except around their maxima. In this region, where a difference in the absolute values of the RPAE and RHF data is observed, the gap between them does not exceed 4.6%, 6.08% and 3.17% for values $\infty, 100$ and 30 of λ_D , respectively. Results of the $3s \rightarrow 6p$ transition GOS for different Debye plasma screening lengths λ_D considered in this study are shown in **Figure 7(c)**. The results in **Figure 7(c)** provide an interesting comparison. In the RPAE-V approach, the peak of the GOS curve for $\lambda_D = 100$ is 1.0747 times lower than that of GOS curve for $\lambda_D = \infty$ and the curve's peak of GOS for $\lambda_D = 30$ is 2.0188 times smaller than the peak of the GOS curve for $\lambda_D = 100$.

In the RHF-V method, the maximum GOS of dipole transition for $\lambda_D = \infty$ is 1.0928 larger than that of the GOS for $\lambda_D = 100$. The maximum GOS for the value 100 was 1.7540 times that of GOS for $\lambda_D = 30$. We note that the magnitude of GOS consistently decreases with decreasing Debye length λ_D .

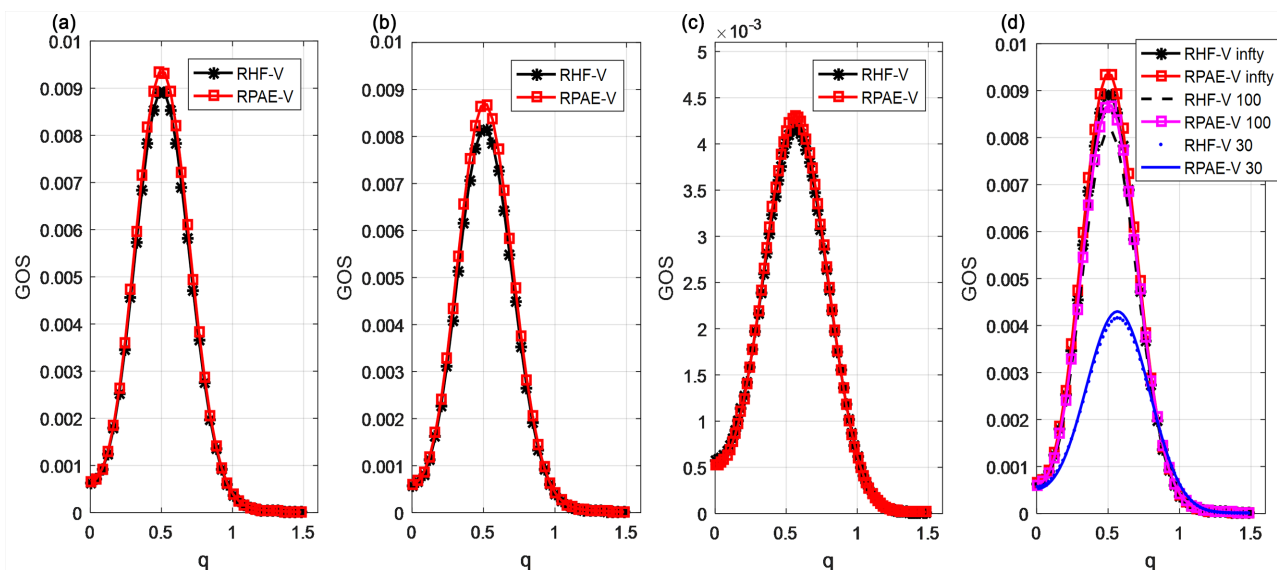


Figure 7. GOS as a function of the transferred momentum q for sodium atom $3s$ to $6p$ transition. In (a), (b) and (c) Comparison of the GOS theoretically calculated in length formulation by Martínez-Flores [7] with that theoretically calculated in present work by using RHF-V and RPAE-V methods. Velocity GOS data for the screened atomic sodium with cases: (a) screening length correspond here to infinity, (b) screening length, (c) screening length. In frame (d), the first two top black curves represent the GOS result for screening length. The second two middle red curves describe the GOS result for screening length while the two lower blue curves correspond to the GOS result for screening length.

Regarding the present investigation of the *GOS*, our results have a considerable effect on the sodium atoms planted in the Debye plasma environment. For $\lambda_D = \infty$, the limiting behavior of the $3s \rightarrow 6p$ transition *GOS* as $q \rightarrow 0$ was also 0.0006412 a.u and 0.0006549 a.u in the present RHF and RPAE velocity calculations, respectively. Both of these values are between the theoretical data of [6] (0.00067) and the theoretical data of [20] (0.000593).

5. Conclusion

In this study, we calculated the velocity form of the *GOS* for dipole transitions of the sodium atom planted in the Debye plasma. The velocity calculations were performed using the method of restrict Hartree-Fock combined with the plasma screening effects and the many electron effects considered in the random phase approximation with exchange. These velocity results prove that plasma Debye screening reduces the magnitude of *GOS* as the Debye plasma screening length decreases, and the electron correlation effects are quite important near the region of the maxima. It is observed that electron correlations hardly manifest in the investigated momentum transfer region where the position of the *GOS* maximum moves to a larger momentum transfer. The RPAE-V results and the theoretical length results [7] are in good agreement, except for the slight difference between them when the momentum transfer is smaller than the values of $q = 0.2, 0.04206$ and 0.5055 a.u for excitation to 3p, 4p and 5p respectively. With the RHF-V results, we also note the same slight difference with those in reference [7] in addition to the discrepancy between them around the position of some maxima. This work also adds new data on the *GOS* of the sodium atom transitions to previous data on other transitions. Comparisons with other theoretical or experimental data would be useful to test the accuracy of the present theoretical calculations performed in the velocity formulation.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

- [1] Han, X.Y., Li, Y.M., Yan, J. and Zhu, L.F. (2009) The Generalized Oscillator Strengths for Na: Monopole, Dipole and Quadrupole Transitions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **42**, Article 195003. <https://doi.org/10.1088/0953-4075/42/19/195003>
- [2] Li, H.W. and Kar, S. (2012) Polarizabilities of Li and Na in Debye Plasmas. *Physics of Plasmas*, **19**, Article 073303. <https://doi.org/10.1063/1.4739229>
- [3] Li, H., Kar, S. and Jiang, P. (2012) Calculations of Dynamic Dipole Polarizabilities of Li and Na Atoms in Debye Plasma Using the Model Potential Technique. *International Journal of Quantum Chemistry*, **113**, 1493-1497. <https://doi.org/10.1002/qua.24347>
- [4] Han, X., Li, Y., Zhang, H., Yan, J., Li, J.M. and Voky, L. (2008) *R*-Matrix Treatment

- of High-Energy Electron-Impact Excitation Processes: The Generalized Oscillator Strengths for the Na $3s-3p$ and $2p-3s$ Transitions. *Physical Review A*, **78**, Article 052702. <https://doi.org/10.1103/PhysRevA.78.052702>
- [5] Chen, Z. and Msezane, A.Z. (2000) Generalized Oscillator Strength for the Na $3s-3p$ Transition. *Physical Review A*, **61**, Article 030703. <https://doi.org/10.1103/PhysRevA.61.030703>
- [6] Qi, Y.-Y. and Ning, L.-N. (2014) Dynamic Processes and Polarizability of Sodium Atom in Debye Plasmas. *Physics of Plasmas*, **21**, Article 033301 <https://doi.org/10.1063/1.4867060>
- [7] Martínez-Flores, C. (2020) Generalized Oscillator Strengths for the Ground State $[2p^63s]^2S$ of Sodium Atom Embedded in a Plasma Medium. *Chemical Physics*, **535**, Article 110759. <https://doi.org/10.1016/j.chemphys.2020.110759>
- [8] Thiele, R., Son, S., Ziaja, B. and Santra, R. (2012) Effect of Screening by External Charges on the Atomic Orbitals and Photoinduced Processes within the Hartree-Fock-Slater Atom. *Physical Review A*, **86**, Article 033411. <https://doi.org/10.1103/physreva.86.033411>
- [9] Bunjac, A., Popović, D.B. and Simonović, N.S. (2017) Resonant Dynamic Stark Shift as a Tool in Strong-Field Quantum Control: Calculation and Application for Selective Multiphoton Ionization of Sodium. *Physical Chemistry Chemical Physics*, **19**, 19829-19836. <https://doi.org/10.1039/c7cp02146a>
- [10] Bethe, H. (1930) Zur Theorie des Durchgangs schneller Korpuskularstrahlen durch Materie. *Annalen der Physik*, **397**, 325-400. <https://doi.org/10.1002/andp.19303970303>
- [11] Amusia, M.Y. and Chernysheva, L.V. (1997) Computation of Atomic Processes A Hand-Book for ATOM Programs. Institute of Physics Publishing.
- [12] Gomis, L., Hibbert, A., Diallo, S., Faye, I.G., Tall, M.S., Diedhiou, I., *et al.* (2014) Generalized Oscillator Strengths for Dipole and Octupole $3p \rightarrow (3d, 4d, 5d)$, Quadrupole and Hexadecapole $3p \rightarrow 4f$ Transitions of Argon Atomic in the Length and Velocity Formulations. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **47**, Article 225207. <https://doi.org/10.1088/0953-4075/47/22/225207>
- [13] Amusia, M.Y. and Chernysheva, L.V. (2021) Computation of Atomic and Molecular Processes: Introducing the ATOM-M Software Suite. Springer. <https://doi.org/10.1007/978-3-030-85143-9>
- [14] Gomis, L., Faye, I.G., Diallo, S., Tall, M.S., Diedhiou, I., Hibbert, A., *et al.* (2015) Length and Velocity Form Calculations of Generalized Oscillator Strengths of Dipole, Quadrupole and Monopole Excitations of Argon. *Physica Scripta*, **91**, Article 015401. <https://doi.org/10.1088/0031-8949/91/1/015401>
- [15] Amusia, M.Y., Chernysheva, L.V., Felfli, Z. and Msezane, A.Z. (2007) Octupole Contributions to the Generalized Oscillator Strengths of Discrete Dipole Transitions in Noble-Gas Atoms. *Physical Review A*, **75**, Article 062703. <https://doi.org/10.1103/physreva.75.062703>
- [16] Bielschowsky, C.E., Lucas, C.A., de Souza, G.G.B. and Nogueira, J.C. (1991) Generalized Oscillator Strength for the $3s-3p$ and $2p-3s$ Transitions in the Sodium Atom. *Physical Review A*, **43**, Article 5975. <https://doi.org/10.1103/physreva.43.5975>
- [17] Buckman, S.J. and Teubner, P.J.O. (1979) Differential Cross Sections for the Electron Impact Excitation of the $3^2P_{1/2,3/2}$ Resonance Levels of Sodium. *Journal of Physics B: Atomic and Molecular Physics*, **12**, 1741-1750. <https://doi.org/10.1088/0022-3700/12/10/020>
- [18] Younis, W.O., Allam, S.H. and El-Sherbini, T.H.M. (2005) Energy Levels and Oscil-

lator Strengths of Excited States in Sodium and Sodium Like Ions. *Proceedings of the Seventh Radiation Physics and Protection Conference (RPC-2004)*, Ismailia, 27-30 November 2004, 17-26.

- [19] Wiese, W.L., Smith, M.W. and Glennon, B.M. (1969) Atomic Transition Probabilities. U.S. Govt. Printing Office, Washington, DC.
- [20] Kelleher, D.E. and Podobedova, L.I. (2008) Atomic Transition Probabilities of Sodium and Magnesium. A Critical Compilation. *Journal of Physical and Chemical Reference Data*, **37**, 267-706. <https://doi.org/10.1063/1.2735328>