

# Generalized Oscillator Strength of Valence-Shell Excitations of Atomic Sodium in Debye Plasma Within the Frame of Two Various Methods

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**How to cite this paper:** Diatta, C., Gomis, L., Faye, I.G., Martinez-Flores, C., Tall, M.S., Diouf, Y., Gomis, R., Coulibaly, M. and Diedhiou, I. (2024) Generalized Oscillator Strength of Valence-Shell Excitations of Atomic Sodium in Debye Plasma Within the Frame of Two Various Methods. *Open Journal of Applied Sciences*, 14, 3649-3667.  
<https://doi.org/10.4236/ojapps.2024.1412239>

**Received:** November 25, 2024

**Accepted:** December 24, 2024

**Published:** December 27, 2024

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## Abstract

The generalized oscillator strengths (GOSs) of  $2p^63s^0$  ( $3p$ ,  $4p$ ,  $5p$ ,  $6p$ ) states excited from sodium ground state in Debye plasma, are studied by two kinds of theoretical approaches: the restricted Hartree-Fock (RHF) method and the random phase approximation with exchange (RPAE). Wavefunctions of the ground state and the excited states are calculated numerically from the RHF equation, employing the local density approach for exchange interaction including, in extension, plasma screening effects. The GOSs have been computed by using these wavefunctions. The results of RHF and RPAE calculations of the GOS for different Debye lengths have been reported for sodium dipole excitation to  $3s^0$  ( $3p$ ,  $4p$ ,  $5p$ ,  $6p$ ). We show, in this study, that RPAE results for values of Debye length  $D = 30, 100, \infty$  are in excellent agreement with those found by other authors. The results of RPAE calculations show that correlation effects are quite significant around the maxima GOS for the excitations to  $3s^0$  ( $4p$ ,  $5p$ ,  $6p$ ) but are found to have no great influence in the GOS for the dipole excitation to  $3s^03p$ . We find that the amplitude of the GOS has noticeably been reduced in going from higher to lower Debye length. We've observed here that the peak of the GOS shifts towards a small momentum transfer when the value  $D = 20$  a.u is taken. These results show an important influence of the Debye plasma screening interactions on the GOS as the screening Debye length is decreased.

## Keywords

Generalized Oscillator Strength, Length Form, Restricted Hartree-Fock, Random Phase Approximation with Exchange, Debye-Hückel Plasma, Screening Effect

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## 1. Introduction

In the present work, we focus on the fast electron inelastic scattering which we characterize by the generalized oscillator strength (GOS). This GOS [1]-[3] concept introduced by Bethe in atomic physics [1] provides information on the valence shell excitations of atoms and molecules. Interest in sodium atom in this study is related to its existence in the atmosphere and for its hydrogenlike electronic structure [4]. It widely exists in comets and stellar wind; it has attracted numerous interests of theoretical and experimental studies [5] [6]. To best of our knowledge, the study of free sodium atom has received main attention by many authors [7]-[9]. From the study in Debye plasma [10]-[20], modifications of various atomic structure and spectrum parameters have been exhibited by using different types model potentials describing the screened interelectronic interactions when solving the Schrödinger equation. Janev *et al.* [10] provide, in their review a comprehensive overview of the fundamental theoretical studies of atomic physics in Debye plasmas modeled with screened interactions. As we know, Murillo *et al.* [11] have focused on the approach which can readily incorporate level shifts of the target as well as dynamic plasma effect before computing dipole oscillator strengths for atomic transitions in such potentials. Photoionization of hydrogen atom and helium  $\text{He}^+$  ion in Debye plasmas have been studied by Li *et al.* [12] by considering the exponential-cosine-screened Coulomb and screened Coulomb (Yukawa) potentials. Taking advantage of the complex coordinate rotation method, Sahoo *et al.* [13] have studied the influence of plasma on photoionization of atomic helium by means of the Debye Hückel model, that incorporates the effects of plasma. Mukherjee *et al.* [14] have shown the dependence of the energies of excited states of helium-like atoms embedded in plasma on both nuclear and Debye parameter. Investigation of oscillator strength, critical screening constant and polarizability of hydrogen-like plasma under Endohedral cavity has been made by Saptarshi *et al.* [15].

By examining the competing effect of plasma charge density and temperature in weakly and strong coupled plasma, Mukherjee *et al.* [16] reported their calculated results of the oscillator strength and polarizabilities for considering 1s, 2s states of the H-like ions embedded in astrophysical plasmas. Using the relativistic treatment, Bahar [17] investigated energy spectrum, transition energies and oscillator strengths for atoms systems Li, Na and K in the presence of quantum plasma environment, under the influence of spherical encompassment and external field. Bahar also elucidated the effect of interaction parameters on the afore-mentioned

observables with details analyses such as alternatives to each other, dominance, optimal ranges or critical values been carrying out. Recently, Bahar [18] has conducted the theoretical investigation on the persistent orbital charge-currents and induced magnetic field of Li and Na atom compressed by spherical confinement, embedded in a quantum plasma. Yue-Ying Qi *et al.* [19] reported their theoretical results of oscillator strengths and dipole polarizabilities of the 3s and 3p states of the sodium. The structure, dipole and generalized oscillator strengths of helium atoms in a plasma have been investigated by Martinez *et al.* [20] with the wavefunctions obtained by using the Debye-Hückel screened (DHS) potential and a more general exponential-cosine screened Coulomb (ECSC) potential when solving the Schrödinger equation in a restricted Hartree-Fock method. In the case of the GOS for ground state  $2p^63s$  of sodium atom, theoretical work of Martínez-Flores [21] has been reported in the literature. This work has been carried out by using wavefunctions obtained with the pseudo-potential model modify the 3s valence in order to obtain the associated GOS. A report of this investigation stimulated full-electron studies of sodium atom in Debye-plasma where the inner electron exchange contributions are significant to account for generalized oscillator strengths of electronic excitations.

In order to supplement this previous work, two approaches have been proposed to take into account the screening interaction of many electron systems. It means here the inclusion of screening of the electron-electron interaction of sodium atoms in plasma studies. One of these methods is the Restricted Hartree-Fock (RHF) method which simplifies the exact Hartree-Fock one in screening environment investigations. This RHF approach has been fruitful in treating screening effect problems in two electron system structure and spectrum parameters with satisfactory results. An example is due to Martinez *et al.* [22] who investigated the effects of plasma on dipole and generalized oscillator strengths of helium. However, to the best of our knowledge, it appears that the influence of plasma environment on the energy levels and the dipole and generalized oscillator strengths of multi electron atomic sodium has not received little attention to date by means of the investigation within the framework of this RHF method.

In the other hand, we also point out here the application of another technique of many electron problems. The specificity of the present method is the way that it takes into account virtual excitations of electrons from other subshells. This approach differs from the common calculations in the fact that we directly obtain the GOS without constructing first a pair of eigenfunctions from an integral equation which describes the collective multi-electron effects. To date no study of GOS has also been conducted on fast charged particle-sodium scattering for excitation process in plasma environment by using this second approach which is the random phase approximation with exchange (RPAE). The aim of the paper is to study in length form, the GOS of sodium atom planted in plasma environment both in the Restrict Hartree-Fock method and the Random Phase Approximation with Exchange approach. Furthermore, the present opportuneness of this study is that

comparison may be made between our results and the earlier provided benchmark results in the reference [21].

This work is organized as follows. Section 2 summarizes the procedure to find atomic orbitals with the Schrödinger equation in a restricted Hartree-Fock (RHF) approach to account for the sodium atom in a Debye plasma. The length formulation of GOS in the modified Hartree - Fock method and in the random phase approximation with exchange one, is the topic of Section 3. We provide, in the Section 4, the GOS results and make comparison with other work where it is possible. We draw the conclusion in the last section. Throughout the present paper, results are given in atomic units, unless explicitly indicated otherwise.

## 2. Computational Method Wavefunctions

To study the GOS of the sodium atom in the inelastic scattering taking place in the presence of Debye-plasma, one needs to calculate the wavefunctions in the initial and final states. In order to investigate the effects of Debye-plasma on these wavefunctions, the radial Schrödinger equation for sodium atom in weak plasma can be written as [22]

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

Here  $\varepsilon_{n\ell}$  is orbital energy;  $V_{eff}^D(r)$  is the sum of the Debye-screened coulomb potential of a nuclei of charge  $Z$  that interacts with electron, the total interaction electron-electron Debye-screened coulomb potential and the Debye-screened exchange potential.

In this paper, we use the Debye-screened exchange potential which is approximated by a statistical free-electron expression with a Thomas-Fermi screening corrections [23] [24]. Then the value of the effective potential  $V_{eff}^D(r)$ , including the Debye screening tends towards zero as  $r$  becomes larger [25]. In the Latter's [23] [24] procedure, the asymptotic behaviour of the effective potential was corrected at large values of  $r$  from atomic nucleus.

The form of the effective potential  $V_{eff}^D(r)$  for the field in which the electron moves can now be written as:

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

if  $r < r_0$  and

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

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  $\sum_{n\ell} N_{n\ell}$ .

Let us note that  $D$  and  $F(\alpha)$  in Equation (2) are respectively the screening length of a Debye plasma and the screening function. This screening function is a correction factor which is equal to [22]-[24].

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

where  $\alpha = \frac{k_s}{k_F} = \frac{1}{Dk_F}$  is defined as the ratio of the Debye screening parameter

$k_s \equiv \frac{1}{D}$  and the fermi momentum  $k_F$ . As can be expected from its formulae there is no screening for  $k_s = 0$  (*i.e.*  $D \rightarrow \infty$ ). With the spherically average total

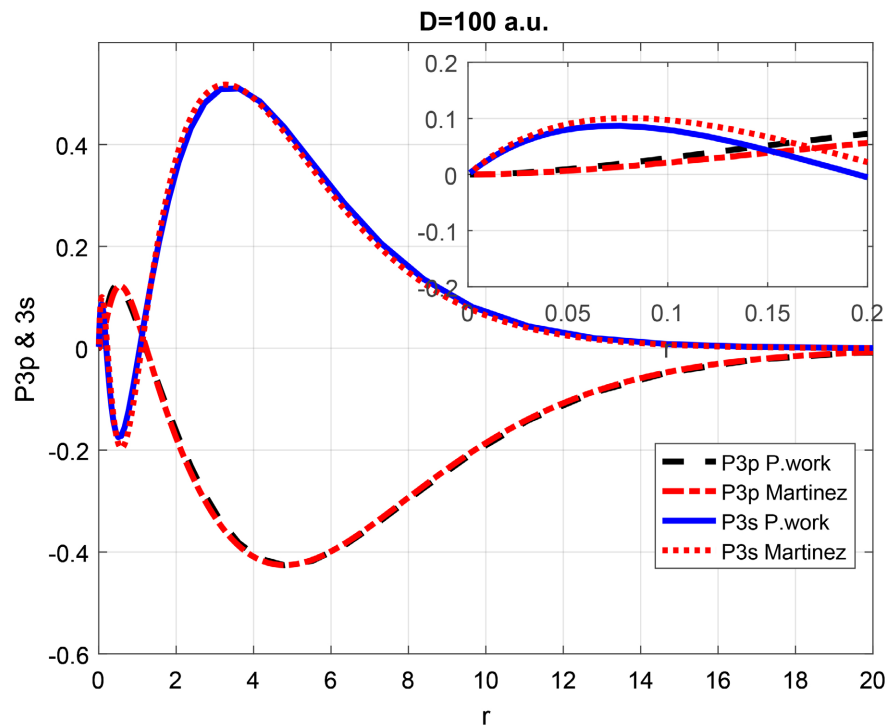
electronic charge density, we set  $\alpha$  equal to  $0.646 \times \left[ \sum_{n\ell} \frac{N_{n\ell} [P_{n\ell}(r)]^2}{4\pi r^2} \right]^{-1/6}$ . It

can be seen in the Equation (2),  $I_{1/2}(r)$  and  $K_{1/2}(r)$  which are obtained by using the modified Bessel functions of first kind  $I_{k+1/2}(r)$  and second kind  $K_{k+1/2}(r)$ , respectively for the case of  $k = 0$ .

In our previous development of unscreened modified Hartree-Fock method, we have used the method applied in a previous paper [26] based on finite difference approximations to numerically calculate the orbital energies and radial wavefunctions with good efficiency. Those orbital energies and radial wavefunctions and related physical quantities as generalized oscillator strengths (GOS) have been obtained for free neon atom [26]. The extension of unscreened numerical modified Hartree-Fock method to screened atomic sodium is a natural choice due to its simplicity and successfully previous usage. The radial wavefunctions for orbital eigen energy are numerically obtained by solving the modified non-relativistic HF Equation (1). In the present case, we have linearized this basic equation and calculated the radial integrals by the quadrature method. The Matlab Software has been used to compute the present data of sodium atomic structure. To test the quality of these radial wavefunctions of atomic sodium in Debye plasma, for example  $D = 100$ , our present radial functions  $P_{3s}$  ground state and  $P_{3p}$  excited state are given in **Figure 1** below and compared with the results provided by [21] where they used the pseudo-potential model approach. The inset graph, in the **Figure 1** shows in detail the behaviour of 3s orbital ground state and 3p orbital excited state for each curve at small radius between 0 and 0.2 a.u.

We have found the other elaborate radial wavefunctions by using the same procedure and the obtained results are used to compute some dipole and GOS for excitation of an atomic sodium in Debye plasma environments.

The present results are those obtained by solving the Equation (1) with the screened modified Hartree-Fock method.



**Figure 1.** Solid and dashed curves describe, respectively, sodium atomic  $P_{3s}$  and  $P_{3p}$  radial wavefunctions of our calculations in Debye plasma. Dotted and dash-dotted curves represent, respectively,  $P_{3s}$  and  $P_{3p}$  data using in [21].

### 3. Length form Evaluation of GOS

Since it has been introduced by Bethe [1] [27] and reviewed by Inokuti [3], the generalized oscillator strength is previously an important property of a free atom. However, we learn from the physical nature of the plasma environment, that the properties of the atom in plasma can differ significantly from those of a free atom. Apart from the other properties, we have used here the generalized oscillator strength to describe the process of interaction between an incident particle and an atom embedded in plasma environment. In the case of the Debye plasma, this concept of generalized oscillator strength for excitation is defined in terms of the energy transfer  $\omega$ , momentum transfer  $q$ , initial state atomic wavefunction  $\Psi_i$  and a particular atomic excited state wavefunction  $\Psi_f$  as [1] [28]:

$$G_{if}(\omega, q) = \frac{2\omega}{q^2} \left| \sum_{j=1}^N \int \Psi_f(\mathbf{r}_1 \mathbf{r}_2 \dots \mathbf{r}_N) e^{iq \cdot \mathbf{r}_j} \Psi_i(\mathbf{r}_1 \mathbf{r}_2 \dots \mathbf{r}_N) d\mathbf{r}_j \right|^2 \quad (5)$$

where  $\mathbf{r}_j$  is vector position of atomic electron  $j$  and  $\exp(i\mathbf{q} \cdot \mathbf{r}_j)$  the interaction operator of this electron with the incident charge particle, in the length formulae calculated in the early work of Bethe.

In carrying out the present restricted Hartree-Fock approach, the atomic wavefunctions  $\Psi_{if}$  are the Slater determinant of spin orbitals which satisfies the antisymmetry property. Taking into account the normalization and orthogonality conditions in integration procedure, Equation (5) is reduced to the sum of the

GOS term describing the transition of one electron to a particular excited state after interaction with the incident particle while other atomic electrons remain in their states. Then, the inelastic collision GOS term of an atomic sodium in Debye plasma for this one electron transition from an initial state denoted by  $m$  to the final state denoted by  $t$  is given by [29]

$$g_{mt}(\omega, q) = \frac{2\omega}{q^2} \left| \int \psi_t(\mathbf{r}) e^{iq \cdot \mathbf{r}} \psi_m(\mathbf{r}) d\mathbf{r} \right|^2 \quad (6)$$

The exponent  $e^{iq \cdot \mathbf{r}}$  in Equation (6) can be expanded into the following series [30]

$$e^{iq \cdot \mathbf{r}} = \sum_{k=0}^{\infty} (2k+1) j_k(qr) P_k(\cos \theta) \quad (7)$$

Here  $j_k(qr)$  is the spherical Bessel function of the first kind of order  $k$ . Taking into account the spherical symmetry of the system, Equation (6) with the help of (7) simplifies considerably after integrating it over the angles, summing over the spin projection and orbital angular momentum in the final state, and averaging it in the initial state. Then the expression of Equation (6) is reduced to the following relation [28]:

$$g_{mt}(\omega, q) = \sum_k g_{mt}^k(\omega, q) \quad (8)$$

where the length form multipole GOS is given by

$$g_{mt}^k(\omega, q) = \frac{2\omega N_m (2k+1)}{q^2 (2\ell_m + 1)} \left| \sqrt{(2\ell_t + 1)(2\ell_m + 1)} \begin{pmatrix} \ell_t & k & \ell_m \\ 0 & 0 & 0 \end{pmatrix} \right. \\ \left. \times \int_0^{\infty} P_{n_m \ell_m}(r) j_k(qr) P_{n_t \ell_t}(r) dr \right|^2 \quad (9)$$

with  $N_m$  the number of electrons in the excited state,  $P_{n_m \ell_m}(r)$  and  $P_{n_t \ell_t}(r)$  being respectively, the final and initial normalized radial functions of RHF wavefunctions. Note that the total angular momentum  $k$  of the electron-hole pair, satisfies the triangular rule  $|\ell_m + \ell_t| \geq k \geq |\ell_m - \ell_t|$ .

According to Equation (9), the GOS can be studied in estimating only the influence of the Debye plasma on sodium atomic structure and the direct excitation of the atomic electron under consideration. In reality, the interaction in a sodium atomic electron involves many electrons simultaneously. In order to obtain a better mathematical treatment of the effects of the dynamical perturbation of the self-consistent field by the fast incoming charged particle, we have adopted an approach based on a collective description of the interaction between atomic electrons. The main idea of this approach is to represent the amplitude transition as a combination of the direct and exchange matrix elements of the inter-electron interaction. The theoretical calculations including the mechanism due to the electron-electron interaction is taken into consideration here within the random phase approximation with exchange (RPAE) [28] [30]. We proceed to calculate the GOS by using the following matrix element defined in RPAE length formulation [28] [30]

$$\begin{aligned}
& \langle \psi_t(r) | L^{RPAE}(\omega, q) | \psi_m(r) \rangle \\
&= \langle \psi_t(r) | e^{iqr} | \psi_m(r) \rangle + \left( \sum_{n \leq F, k \geq F} - \sum_{k \leq F, n \geq F} \right) \frac{\langle \psi_k(r') | L^{RPAE}(\omega, q) | \psi_n(r') \rangle}{\omega - \varepsilon_k + \varepsilon_n + i\alpha(1 - 2\beta_k)} \quad (10) \\
& \quad \times \langle \psi_n(r') \psi_t(r) | V | \psi_k(r') \psi_m(r) \rangle
\end{aligned}$$

where  $\langle \psi_n(r') \psi_t(r) | V | \psi_k(r') \psi_m(r) \rangle$  stands for the combination of the direct and exchange matrix elements of the electron - electron interaction  $\psi_k(\psi_n)$  is the final (initial) virtual excitation state with their corresponding final (initial) orbital energy  $\varepsilon_k(\varepsilon_n)$ .  $F$  is the Fermi level of the sodium atom and the Fermi step function  $\beta_k$  looks as follows: for unoccupied states  $\beta_k = 0$  and for occupied states  $\beta_k = 1$ . The complex number  $i\alpha$  in denominator of Equation (10), with imaginary part  $\alpha \rightarrow 0^+$  just gives us the direction of tracing the pole in integrating.

To incorporate the effects of correlations into the calculation of the GOS, we just use a relation similar to (6). In this new GOS's expression, the factor form is the transition matrix element including the mechanism describing the response of the interacting multielectron atomic sodium given in (10). Therefore, the length form of GOS of the RPAE contribution due to different electron interactions is introduced:

$$g_{mt}^{RPAE}(\omega, q) = \frac{2\omega}{q^2} \left| \int \psi_t(\mathbf{r}) L^{RPAE}(\omega, q) \psi_m(\mathbf{r}) d\mathbf{r} \right|^2 \quad (11)$$

Due to the fact that some terms of the denominators in Equation (10) become zero at  $\omega = \varepsilon_k - \varepsilon_n$  in the calculations, it is difficult to investigate the discrete excitations numerically in accuracy and efficiency. To avoid this singularity at  $\omega = \varepsilon_k - \varepsilon_n$ , it can be derived that the expression of GOS under the procedure described in detail in [31] [32] is in the first non-vanishing order:

$$g_{mt}^{RPAE}(\omega, q) = \frac{|L_{mt}^{RPAE}(\omega, q)|^2}{1 + \sum_{(mt) \neq (kn)} \frac{|V_{mkn}|^2}{(\omega - \varepsilon_k + \varepsilon_n)^2}} \quad (12)$$

where  $L_{mt}^{RPAE}(\omega, q)$  is the regular solution of the Equation (10) at  $\omega = \varepsilon_k - \varepsilon_n$  by dropping the singular terms and  $V_{mkn}$  represents, symbolically, the last factor in Equation (10) which denotes a combination of the direct and exchange matrix elements of the interaction electron-electron

$$V_{mkn} = \langle \psi_n(r') \psi_t(r) | V | \psi_k(r') \psi_m(r) \rangle.$$

The formulas (9) and (12) are reduced to a form suitable for numerical computation in this paper. The results for GOS of valence-shell excitations of atomic sodium in Debye plasma, computed here from these formulas by using Matlab software are presented and compared with those obtained by other authors.

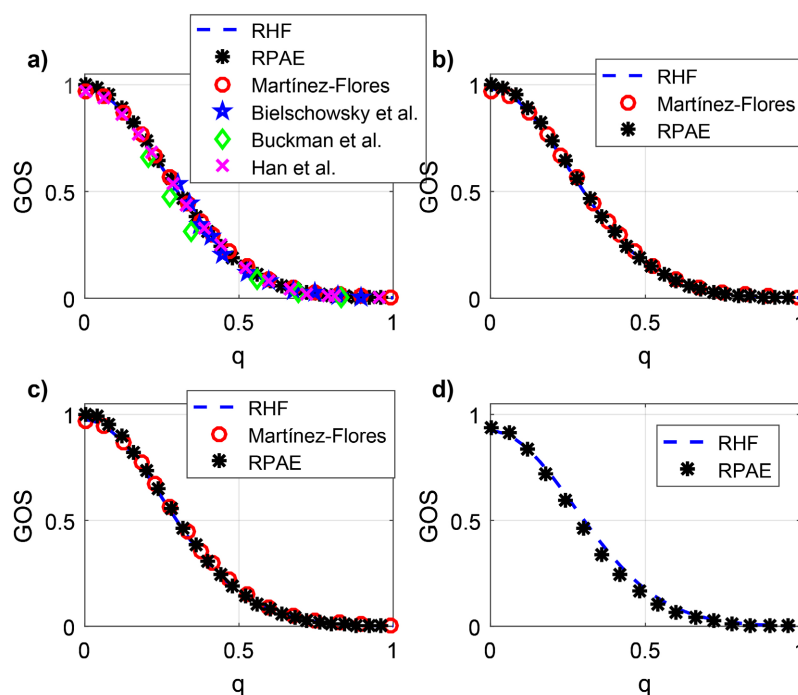
#### 4. GOS of Dipole Excitations and Discussion

The present calculations have been performed for the transitions 3s to 3p, 4p, 5p

and 6p of the sodium atom in Debye plasma. In our calculations, presenting the GOS of these transitions for screening length  $D = \infty, 100, 30$  and  $20$ , appears to work quite well in investigating the competition between shell electron interactions and plasma screening effects and also offers a significant advantage to compare them with available theoretical and experimental data [19] [21] [33].

#### 4.1. Transition of 3s to 3p

We show our findings in **Figure 2** for the dipole GOS for the transition 3s – 3p. These results shown in **Figure 2** are compared with the experimental data given in listed references [6] [33] and those obtained theoretically by others [21] [34] **Figure 2(a)** shows a comparison between the present RHF and RPAE results using the wavefunctions of sodium atom in Debye plasma for  $D = \infty$  and the results of other authors obtained in their theoretical [21] [34] and experimental [6] [33] works. It's seen that our present results agree well with those of the other previous theoretical and experimental works quoted above.

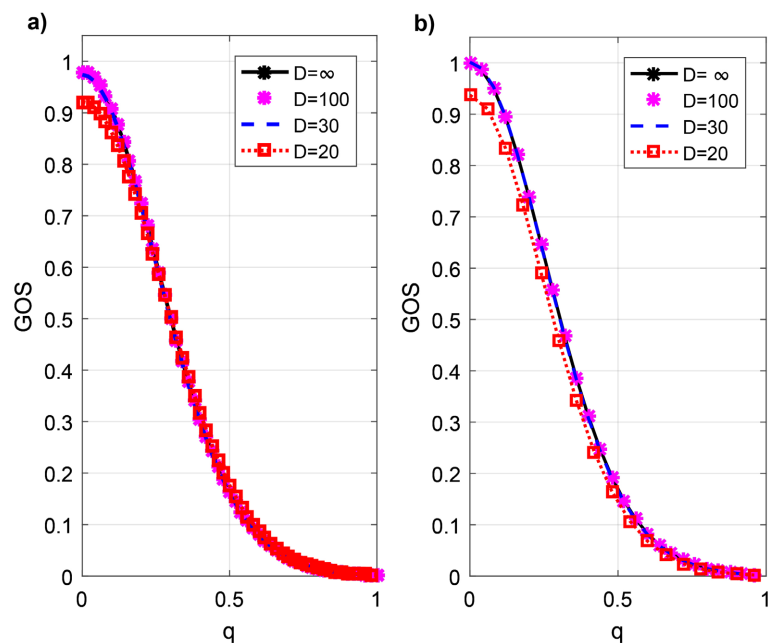


**Figure 2.** Generalized oscillator strength as a function of the momentum transfer  $q$  for sodium atom 3s to 3p transition. In (a) for  $D = 10^{10}$  (infinity), the RPAE (black solid asterisk) and RHF (blue dashed line) results in comparison with the experimentally data by Bielschowsky *et al.* [33] (blue star symbol) and Buckman *et al.* [6] (green diamond symbol), and with those theoretically values of Martínez-Flores [21] (red circle symbols) and Han *et al.* [34] (magenta cross symbols). In (b), for a screening length  $D = 100$  a.u., in (c) for a screening length  $D = 30$  a.u., in (d) screening length  $D = 20$  a.u.

For each screening length  $D$ , the curves of the RHF and RPAE GOS all have the same shape and amplitude in **Figure 2**. This agreement between our RHF and RPAE results may be due to the negligible effect correlations happened into the

transition 3s to 3p. They are in accordance with the data of [21].

We conclude by emphasizing that the plasma environment represented here by the plasma Debye-Hückel screening model has already described successfully the plasma's confining effects, but at the cost of decrease in the interaction between atomic sodium electrons. In all cases in **Figure 2** and **Figure 3** the curves of the GOS decrease as the momentum transfer increases. As seen in the **Figure 3**, GOS curves for  $D = \infty, 100$  and 30 are so close together and are above those describing the calculated data GOS for  $D = 20$ . The agreement between them is satisfactory except for the  $q$  region of 0 - 0.2 a.u. The maximal gap between them is about 5.8% for RHF results in the region where the disagreement is observed in **Figure 3(a)** while it's 6.09% for RPAE results in the **Figure 3(b)**. This difference can be ascribed to the little overlap in the matrix element transition between the main part of the final and initial wave functions which are apparently more sensitive to the increase screening interaction in the region of radial distance close to the coordinate origin. It is found here that, as a consequence of Debye - plasma, the probability for excitation 3s to 3p is reduced as the screening length  $D$  decreases, thus modifying the GOS amplitude. Then, for values of  $D = \infty, 100$  and 30, the GOS value obtained from **Figure 3(a)** as  $q \rightarrow 0$  in RHF method is 0.9796 while it becomes 0.9222 for the screening length  $D = 20$ . From **Figure 3(b)**, a similar situation is observed for the RPAE method but at the three values  $\infty, 100$  and 30 with the GOS equals to 0.9981 and 0.9373 when screening length takes the value 20. For this value  $D = 20$ , the present work as  $q \rightarrow 0$ , slightly underestimates value of oscillator strength found in reference [21].

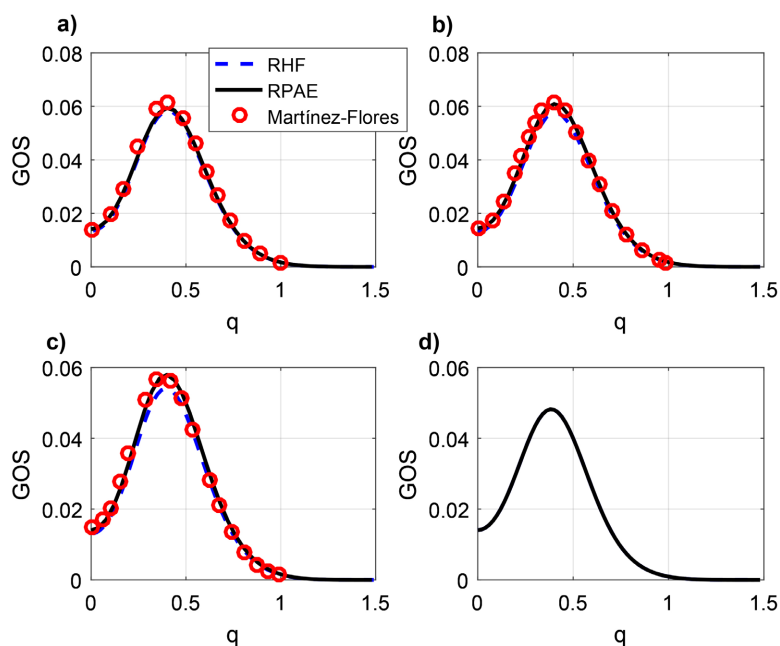


**Figure 3.** Generalized oscillator strength as a function of the momentum transfer  $q$  for sodium atom 3s to 3p transition. The calculations were performed for the values of the screening parameter  $D = 20, 30, 100$  and  $\infty$  a.u. The curves in (a) are the present RHF results while those in (b) are the RPAE findings.

For the other values of GOS there is no theoretical data, in our knowledge, to compare in **Figure 2(c)** our results GOS and the earlier calculation ones for this Debye length value  $D = 20$ . Clearly the free value ( $D \rightarrow \infty$ ) of the RPAE GOS transition  $3s - 3p$  reaches 0.9981 is almost close to the dipole oscillator strength with values of 0.97981 and 0.97976 for Qi *et al.* [19] and Martínez-Flores [21] theoretical results, respectively. The discrepancy between our theoretical value with the measured oscillator strength with value of 0.9820 for Wiese *et al.* [35] does not exceed 1.7%.

## 4.2. Transition of 3s to 4p

**Figure 4** describes the results for the GOS for excitation to 4p of the sodium atom in Debye plasma while **Figure 5** displays them for various values Debye lengths. The GOSs of dipole transition pictures in these figures have qualitatively similar behaviour. The RPAE calculated GOS values agree with the computed results of [21] except when  $q < 0.2$ . In the **Figure 4(a)**, **Figure 4(b)** and **Figure 4(c)**, there is a small difference in absolute values between the results [21] and the present RHF ones as  $q \rightarrow 0$ . We note that the GOS values of the theoretically work of [21] are greater than those calculated by us in the RHF method.

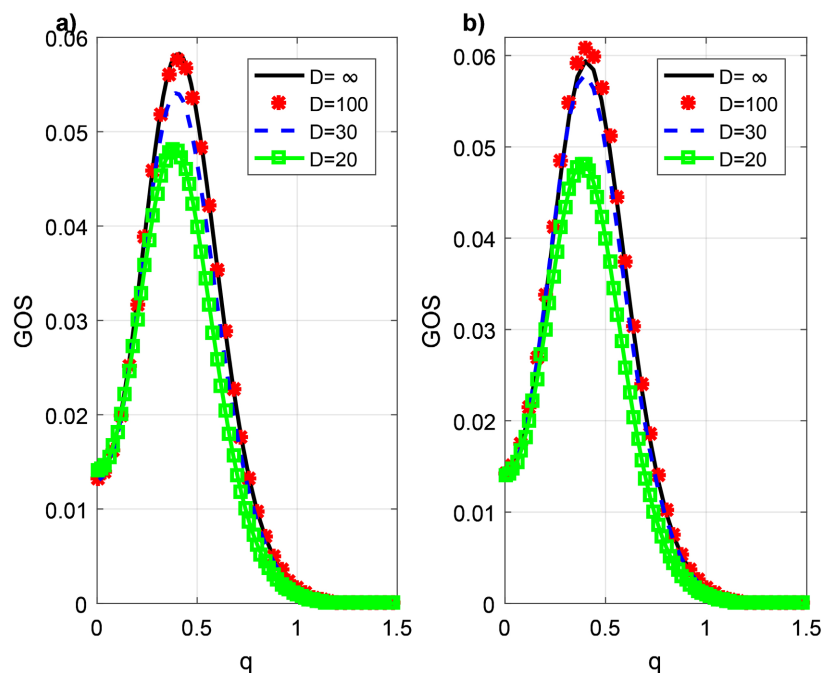


**Figure 4.** Generalized oscillator strength as a function of the momentum transfer  $q$  for sodium atom  $3s$  to  $4p$  transition. We show the RHF (dashed line) and RPAE (solid line) results in comparison with those reported values of Martínez-Flores [21] (red circles) calculated with the pseudo-potential approach. In frame (a), we show values for (a)  $D = 10^{10}$  (infinity) a.u., (b)  $D = 100$  a.u., (c)  $D = 30$  a.u. and (d)  $D = 20$  a.u.

A possible cause for this weak disagreement due to the variation of the wave-functions for small atomic electron radius obtained in the two different calculations. Clearly the peak values of the RPAE GOS are almost the same with those

obtained in the theoretical work of [21].

This agreement should be explained by the fact that the coulomb interelectron interaction effects are weakened by the screening one. It means that the intensity of the interaction due to the screening Debye plasma become more important than the electron-electron interaction describing by the RPAE. The curves of the RPAE approach emphasizes many correlation effects around the maxima where their contribution is about 1.87%, 5.24% and 6.66% for Debye lengths value of  $\infty$ , 100 and 30 respectively. For value of  $D = 20$ , for the GOS of the dipole transition, we observe a minor contribution of correlation effect of the RPAE in comparison with the RHF values. This result demonstrates that, the Debye length decreases with the plasma increasing screening effect. As observed in **Figure 5(a)** and **Figure 5(b)** for the RHF and RPAE results respectively, the amplitude of the GOS of the  $3s \rightarrow 4p$  dipole transition is almost the same for the two values  $\infty$  and 100 of the parameter screening  $D$ . Our theoretical treatment using the RPAE gives the GOS transition  $3s \rightarrow 4p$  reaching a dipole oscillator strength with value of 0.01403. Here, we reported the dipole oscillator strength with values of 0.01423 and 0.01420 for Qi *et al.* [19] and Martínez-Flores [21], calculated results, respectively.



**Figure 5.** Generalized oscillator strength as a function of the momentum transfer  $q$  for sodium atom  $3s$  to  $4p$  transition. The calculations were performed for the values of the screening parameter  $\infty$ , 100, 30 and 20 a.u. The curves in (a) are our RHF results while those in (b) represented our RPAE theoretical data.

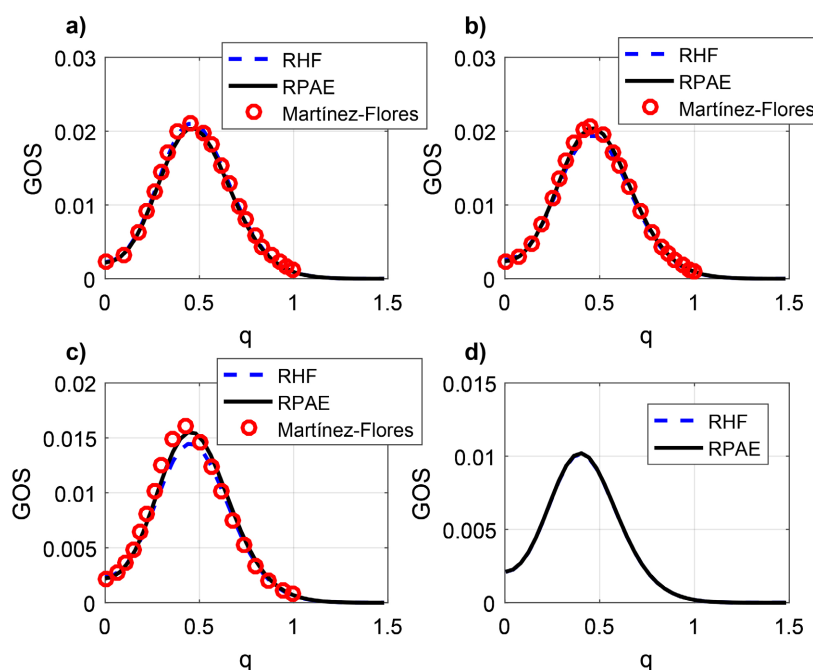
Once again, for free values case ( $D \rightarrow \infty$ ), result from the present work shows a slight difference from that of the previous work of other authors. The disagreement between the present theoretical value with the measured value GOS of

0.0142 for Wiese *et al.* [35] is also less than 1.2%. We note a reduction in amplitude as a selected set of the screening parameter  $D$  is 100, 30 and 20.

In RHF description, the maximum of the GOS of dipole transition obtained for the Debye length  $D = 100$  is 1.0669 larger than the corresponding one for the Debye length  $D = 30$  while this ratio becomes 1.0509 in the RPAE approach. We note that the amplitude of the GOS for Debye screening value 30 is more important than that calculated for the value of  $D = 20$ . The ratio calculated in this case is about 1.2664 in the RHF method while in the RPAE approximation, we obtain 1.3598. It shows that the increasing of plasma strong interactions has a considerable effect on the sodium atom in plasma.

### 4.3. Transition of 3s to 5p

The GOS for the transition  $3s \rightarrow 5p$  is shown in **Figure 6** and compared with the theoretical data found in the work of Martínez-Flores [21]. It is evident from **Figure 6(b)** and **Figure 6(c)** that those RPAE dipole values for sodium atom in Debye plasma environment agree with findings of [21] for  $D = 100$  and 30. For  $D = \infty$ , we note in the **Figure 6(a)** that the RPAE results are slightly less important around the maximum than our calculated RHF data which are in close agreement with the results in the reference [21]. The present work gives the dipole oscillator strength of  $3s \rightarrow 5p$  transition with value 0.002158. This value is in accordance with the value of oscillator strength 0.00216 found by others [19] [21].

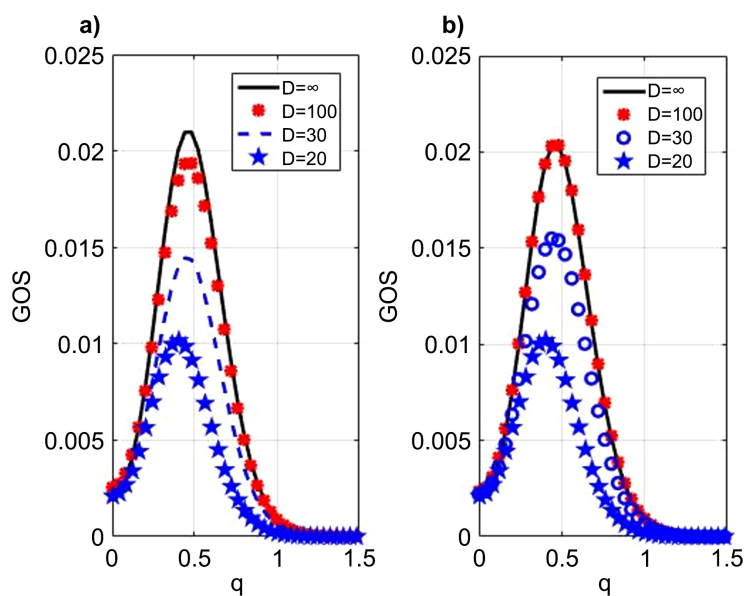


**Figure 6.** Generalized oscillator strength as a function of the momentum transfer  $q$  for sodium atom  $3s$  to  $5p$  transition. We show the RHF (dashed line) and RPAE (solid line) results in comparison with those reported values of Martínez-Flores [21] (red circles) calculated with the pseudo-potential approach. In frame (a), we show values for (a)  $D = 10^{10}$  (infinity) a.u., (b)  $D = 100$  a.u., (c)  $D = 30$  a.u., and  $D = 20$  a.u.

We remark the agreement between these values of theoretical calculations and the value 0.0022 obtained in the experimental work of Wiese *et al.* [35].

The contribution of the correlations introduced by the RPAE approach is about 4.91% and 6.71% in the region of maxima for the Debye lengths  $D = 100$  and  $D = 30$ , respectively. **Figure 6(d)** gives a comparison of the present GOS of dipole transition result of the same transition obtained with  $D = 20$  by using the RHF and the RPAE approaches. For  $D = 20$ , comparison is not made here because no GOS of transition data are available in the literature in best of our knowledge. As shown in this figure, dipole GOS pictures have a same profile with one maximum. It's interesting to note that the RHF GOS magnitude is in good agreement with the RPAE one in the momentum transfer  $q$  region of the present study.

We have plotted in **Figure 7** the variation of the GOS  $3s \rightarrow 5p$  as a function of the momentum transfer  $q$  for the screened case with Debye lengths  $D = \infty$ , 100, 30 and 20 a.u. The RHF and RPAE calculations are presented in **Figure 7(a)** and **Figure 7(b)**, respectively. For Debye lengths  $D = \infty$  and  $D = 100$ , the computed results agree well in the RPAE investigation and slightly differ around the maximum in the RHF calculations with the ratio of 1.104%. It is observed that the curves of the GOS for  $D = 30$  have the same shape but different amplitudes with those obtained for the two values  $\infty$ , 100 of  $D$ . The maximum of GOS of the dipole transition found with  $D = \infty$  and 100 in the RPAE description is 1.335 larger than the corresponding one calculated with  $D = 30$ .



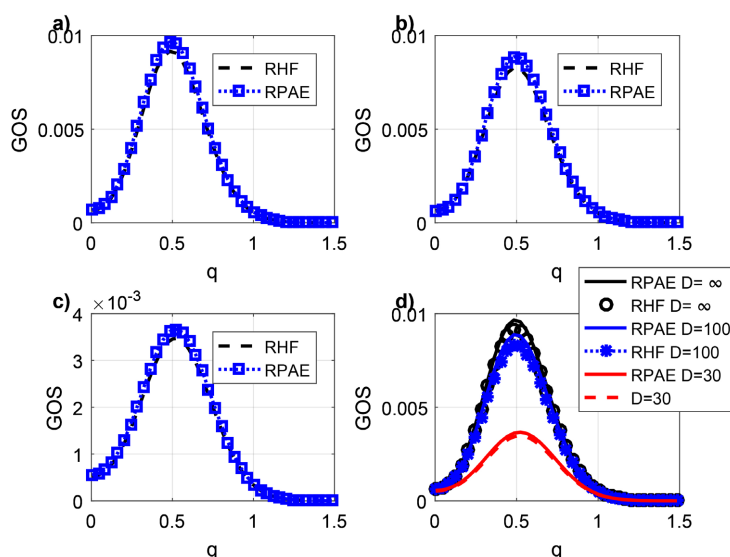
**Figure 7.** Generalized oscillator strength as a function of the momentum transfer  $q$  for sodium atom  $3s$  to  $5p$  transition. The calculations were performed for the values of the screening parameter  $\infty$ , 100, 30 and 20 a.u. The curves in (a) are our RHF results while those in (b) represented our RPAE theoretical data.

In RHF method, the ratio of the amplitude GOS for  $D = \infty$  and 100 that are obtained with  $D = 30$  is respectively 1.478% and 1.339%. The reason has been

reported above and also can be explained as follows: the plasma screening effect makes magnitude of the GOS decreases as the Debye length moves to the smaller values. The important observation in **Figure 7** is that the curves of the GOS  $3s \rightarrow 5p$  transition obtained with  $D = 20$  have the same profile as those found by taking  $D = \infty, 100$  and  $30$ .

The behaviour of this GOS for the screening length  $D = 20$  can be associated with the wave functions extended to the larger radius when the plasma screening lengths approach to a critical  $D$  value given in the reference [19]. This behaviour is an observed decrease in the width of the Gaussian curve. It might be caused by the fact that the matrix element transition given by formula GOS, contains the radial distribution of electron wave functions which become broader and reduced in amplitude with the increasing screening interactions (decreasing value of the Debye length corresponding here to  $D = 20$ ). A closer inspection of **Figure 7** demonstrates that for a given  $D = 20$  the GOS maximum position becomes smaller than those obtained with  $D = \infty, 100$  and  $30$ . So, it should be pointed out that the plasma correlations effect is more pronounced in the case of  $D = 20$ . This brings out that the maximum position of GOS move to a little smaller momentum transfer squared with the stronger effects of the plasma environment (Debye length towards critical  $D$  value) on sodium atomic as has been already noted in [36] by Qi *et al.* in their GOSs investigation of hydrogenlike ions in Debye plasma.

#### 4.4. Transition of 3s to 6p



**Figure 8.** GOS as a function of the momentum transfer  $q$  for sodium atom  $3s$  to  $6p$  transition. In (a), (b) and (c) Comparison of the dipole GOS calculated in RHF method with that obtained in RPAE approach. Computational dipole GOS for the screened sodium atom with cases: (a) screening length  $D = 10^{10}$  correspond here to infinity, (b) screening length  $D = 100$  and (c) screening length  $D = 30$ . In (d), the first two top black curves represent the GOS result for screening length  $D = 10^{10}$ . The second two middle blue curves describe the GOS result for screening length  $D = 100$  while the two lower red curves correspond to the GOS result for screening length  $D = 30$ .

In **Figure 8**, we present results of  $\infty$ , 100 and 30 screening Debye length GOS for the transition  $3s \rightarrow 6p$ . As seen in the **Figure 8(a)**, **Figure 8(b)** and **Figure 8(c)**, the curves of the RHF and RPAE GOS obtained at  $D = \infty, 100, 30$  have the same shape, but their amplitudes differ around the extrema.

The effects of the correlations contribute respectively, at 5.215%, 6.659% and 5.189% around the maximum for these three values  $\infty$ , 100, 30. For the variation of the screening Debye length  $D$ , the RHF and RPAE calculations have both been presented in **Figure 8(d)**. This **Figure 8(d)** illustrates the comparison of our results for different screening lengths. Three curves obtained from the present RHF data and RPAE results at  $D = \infty, 100, 30$  have the same shape. As it has already been revealed for  $3s \rightarrow np$  (with  $n = 3; 4; 5$ ), they present one maximum and decrease until achieving zero above  $q = 1.5$  a.u.

We observe also from **Figure 8(d)** that for the decreasing Debye length the amplitude of GOS of the dipole transition diminishes. The ratio of the amplitude GOS for  $D = \infty$  and  $D = 100$  is about 1.1 as in RPAE and RHF methods. For values 100 and 30 of  $D$ , it is less than 3 in these two methodologies.

## 5. Conclusion

We have investigated both the plasma Debye screening effects and the correlation effects on the GOS of the dipole transition of the sodium atom in plasma environment. The results calculated in both restricted Hartree-Fock and random phase approximation with exchange for the screened sodium discrete excitations from the ground state  $2p^63s^1$  to  $2p^63s^0$  (3p, 4p, 5p, 6p) have proved that the dipole GOS is decreased in going from higher to lower Debye length  $D$ . At  $D = \infty, 100$  and 30; the many-electron effects are mildly quite important only around the region of the dipole GOS maxima of the excitation to  $2p^63s^0$  (4p, 5p, 6p) while they are not significant in the excitation to  $2p^63s^03p$ . The investigation lets us see now the correlation effects estimations are negligible than the plasma Debye screening effects for  $D = 20$  when we apply the RPAE treatment. The new data of the GOS for dipole transition of three excitations considered in the present work have been added for the screening length which may be close to its critical values where transition is no longer bound because the plasma screening interactions become usually stronger. Also, with the present study, the RHF and RPAE calculations give, to the best of our knowledge for the different values of Debye lengths  $D$ , theoretical data of GOS for the transition  $3s \rightarrow 6p$  of Na atom in Debye plasma. So, further theoretical and experiments data are needed to test the accuracy of our RHF and RPAE calculations.

## Conflicts of Interest

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

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