# Be I isoelectronic ions embedded in hot plasma

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The influence of plasma screening on the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^3P_1^o$ intercombination and the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1^o$ allowed transitions is investigated theoretically for several ions along the Be I isoelectronic sequence (C III, N IV, O V, Si XI, Fe XXIII, and Mo XXXIX). For the case of a weakly coupled hot plasma, multiconfiguration Dirac-Fock computations have been carried out for these ions by considering a (time averaged) Debye-Hückel potential for both the "electron-nucleus" and "electron-electron" interaction. The plasma screening is found to enlarge the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^3P_1^o$ excitation energy uniformly along the Be I isoelectronic sequence, leading to an increasing blueshift of this intercombination line as the nuclear charge is increased. For the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1^o$ resonance line, in contrast, the transition energy is either blueshifted *or* redshifted in dependence of the screening parameter and owing to a cancellation of the plasma screening on the electron-nucleus and electron-electron interaction. This interplay of the (external) plasma screening with the internal interactions in the berylliumlike ions leads, for instance, to a shift of the resonance transition from red to blue in going from O V to Si XI ions. Apart from the screening effects on the transition energies, we also investigate their influence on the oscillator strengths and emission rates along the Be I isoelectronic sequence.

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## I. INTRODUCTION

In *hot* plasmas, i.e., an ensemble of atomic ions and electrons, the interactions of the charges are usually modified (screened) by the surrounding ions and fast electrons. Of course, such a screening of the Coulomb interaction of charged particles also alters the electronic transition properties of ions embedded in a plasma, when compared with *free* ions in vacuum. Therefore, the spectral properties of singly or multiple ionized atoms have been found important for the diagnostics of laboratory plasmas or for understanding stellar spectra and atmospheric opacities.

In fact, a large number of computations have been performed during the last decades in order to investigate plasma screening effects on hydrogenlike ions [1–6], heliumlike [7–11], or even many-electron systems [12–15]. In most of these case studies, a Debye-Hückel (type) potential was considered in the framework of the nonrelativistic atomic theory in order to model a *weakly coupled hot* plasma. Relativistic calculations considering different plasma models are also available [16–20]. Bielinska-Waz *et al.* performed a relativistic computation for hydrogenlike ions by using a screened Debye-Hückel potential for the electron-nucleus interaction [19]. These authors showed, in particular, that relativistic corrections on the plasma screening become necessary for the interpretation of the spectra, especially if the lines of multiple-charged ions are to be used in the spectral analysis. Apart from the plasma diagnostics, a proper treatment of the screening effects (potentials) has been found useful also in other areas of physics, such as nuclear and elementary particle physics [21], solid state physics [22], or even the design of nanostructures [23,24]. In these applications, many-electron ions often occur and require one to describe both the electron-nucleus and electron-electron interaction within a proper relativistic framework, especially if highly ionized species are involved.

In the present work, the influence of the plasma screening is investigated for the berylliumlike C III, N IV, O V, Si XI, Fe XXIII, and Mo XXXIX ions in the framework of the multiconfiguration Dirac-Fock (MCDF) theory. To include these plasma effects in the computations, a screened Debye-Hückel potential has been incorporated for both the electron-electron and the electron-nucleus interaction in the ions. In particular, emphasis was placed on the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1^o$ allowed and the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^3P_1^o$ intercombination transitions between the low-lying levels of the berylliumlike ions. Since the intensity ratio of the resonance to the intercombination line is known to be very sensitive to the electron density (near to the nuclei), this ratio has been found a powerful tool for the analysis of *hot* plasmas, such as solar and stellar atmospheres [25–27]. Moreover, the intercombination lines have been utilized also for the plasma diagnostics of tokamak plasmas [28]. Overall, the resonance and intercombination lines from the berylliumlike ions have been observed in a wide variety of astrophysical and laboratory plasmas [29]. Fe XXIII ions, for instance, were observed not only in fusion plasmas but also in the corona and the flares of the sun [30] as well as in intragalactic gas [31].

To describe the effects of the plasma screening on the spectral properties of berylliumlike ions, relativistic atomic computations have been carried out self-consistently for a wide range of screening parameters. Since the plasma screening is proportional to $(n_e/T_e)^{1/2}$, where $n_e$ denotes the density and $T_e$ is the temperature of the plasma, the variation of the energy and strength of atomic transitions can be used

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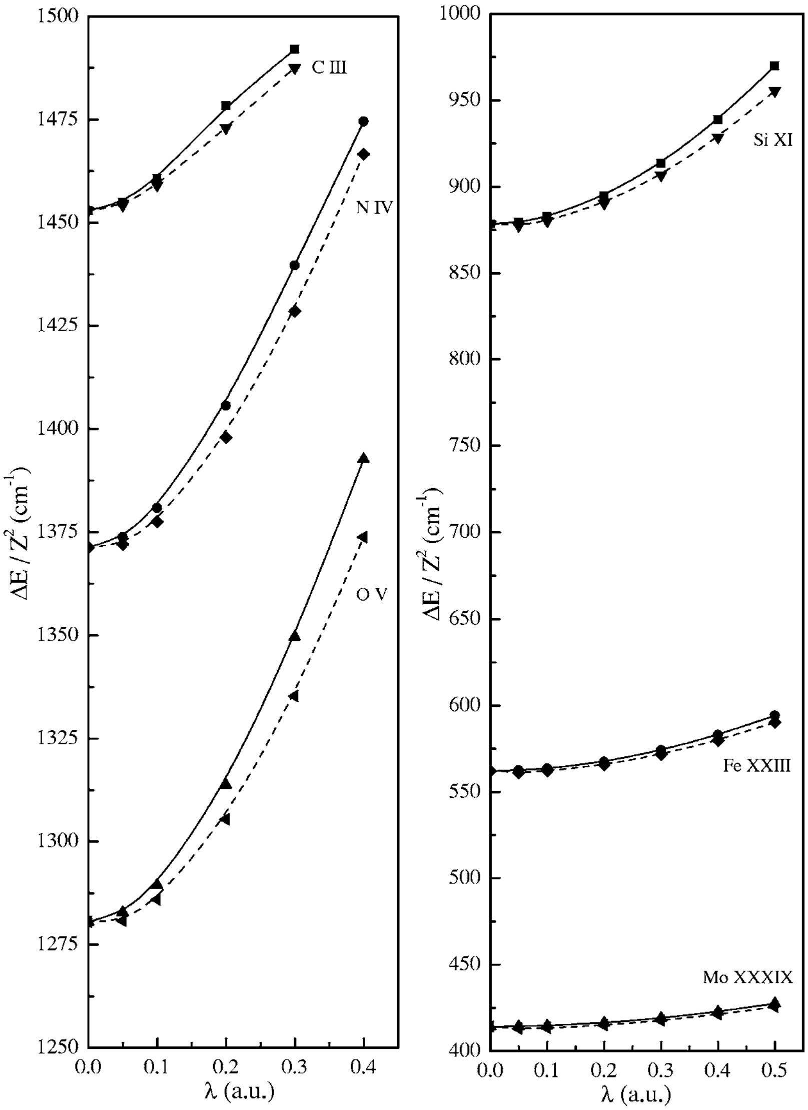


FIG. 1. Excitation energies (scaled by $Z^{-2}$) for the $2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^3P_1^o$ intercombination transition as function of the plasma screening parameter λ. Results are compared for screening only the electron-nucleus interaction (solid line) and for screening both the electron-nucleus and the electron-electron interaction (dashed line).

in the diagnostics of plasmas in order to derive information about its properties and time evolution. In Sec. II, we briefly describe the use and consequences of a Debye-Hückel potential in relativistic atomic MCDF calculations, while the computational details are outlined in Sec. III. Detailed calculations have been carried out for the low-lying $2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^{1,3}P_1^o$ transitions in dependence on the plasma strengths. Section IV shows the results in details and the discussion on the influence of plasma screening on the excitation energy and oscillator strengths along the sequence. In particular, these calculations demonstrate that the Debye-Hückel screening should be incorporated into both the electron-nucleus and electron-electron interaction, in order to obtain reliable results. Finally, a few conclusions are drawn in Sec. V on the computed results and their applicability to plasma diagnostics.

## II. DEBYE-HÜCKEL MODEL HAMILTONIAN

To describe the effects of the plasma screening on the electronic properties of multiple charged ions, let us consider a "guest" ion with nuclear charge $Z$ which is embedded in a weakly coupled hot plasma. As any charged particle, such an ion attracts the electrons and repels the ions from its nearby plasma neighborhood. However, since the mass of the ions is much larger than those of the electrons, the latter ones move faster and cause a net electric field as seen by the electrons and ions inside the plasma. For a *hot* plasma, therefore, the (pairwise) Coulomb interaction among the charged particles needs to be modified and is best described by means of a Debye-Hückel potential. In atomic units, this potential reads as

$$V^{\mathrm{DH}}(r,\lambda) = -\sum_{i}^{N} \frac{Ze^{-\lambda r_i}}{r_i} + \sum_{i>j}^{N} \frac{e^{-\lambda r_{ij}}}{r_{ij}} = \sum_{i}^{N} V^{\mathrm{DH}}(r_i,\lambda) + \sum_{i>j}^{N} V^{\mathrm{DH}}(r_{ij},\lambda), \quad (1)$$

where $N$ is the number of bound electron, $r_i$ is the distance of the $i$th electron from the nucleus, and $r_{ij}$ the distance between the electrons $i$ and $j$, respectively. Moreover, the

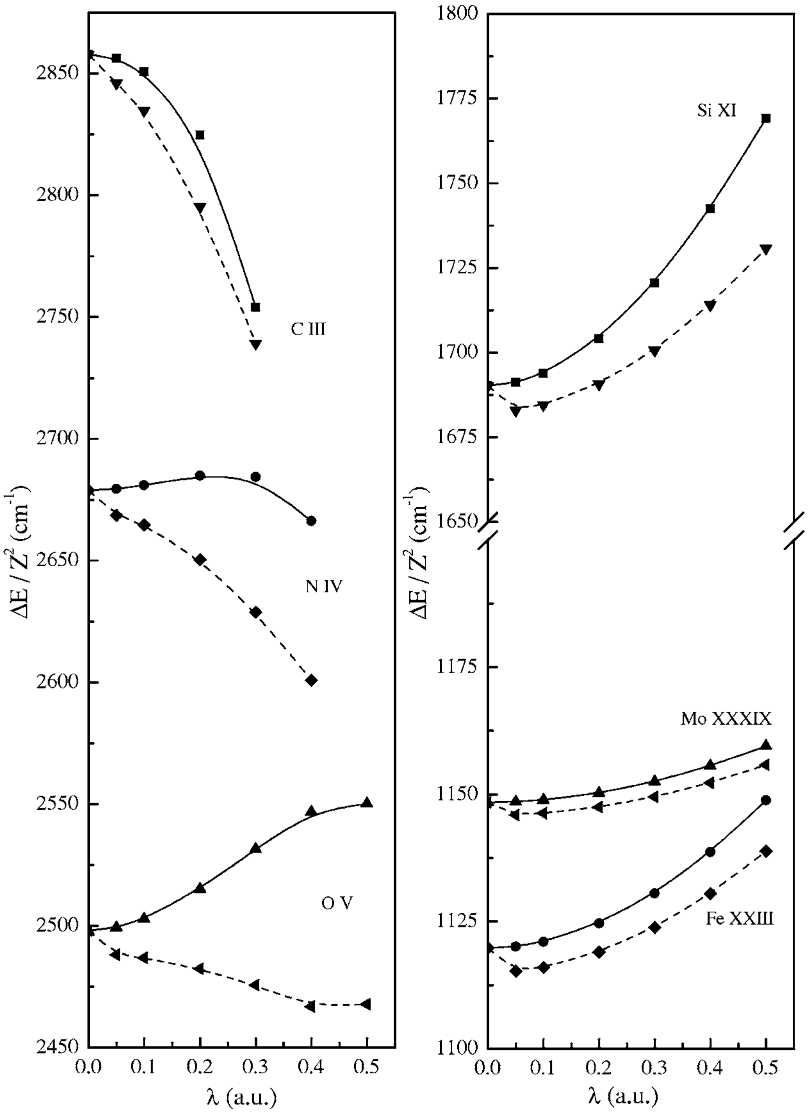


FIG. 2. Excitation energies (scaled by $Z^{-2}$) for the $2s^2\,{}^1S_0 \rightarrow 2s2p\,{}^1P_1^o$ resonance transition as function of the plasma screening parameter λ. See Fig. 1 for details.

plasma screening parameter λ in Eq. (1) is the inverse of the Debye shielding length and can be expressed in terms of the electron density $n_e$ and the temperature $T_e$ of the plasma as

$$\lambda = \left[ \frac{4\pi n_e}{kT_e} \right]^{1/2}, \qquad (2)$$

i.e., any given λ is associated with a certain plasma environment. In the computations below, we shall replace the "electron-nucleus" and "electron-electron" interactions of the ion by the corresponding Debye-Hückel potentials in Eq. (1) and modify the screening by means of the parameter λ.

All the atomic calculations have been carried out within the MCDF model, a generalization of the common Dirac-Fock formalism for describing bound many-particle systems. This model for the electronic structure of atoms and ions has been implemented, for instance, in the GRASP92 [32] and the RATIP codes [33] and has been found very useful to incorporate both the effects of relativity and correlations within the same computational framework. Usually, the nucleus is assumed to be stationary and is modeled either as a pointlike or extended charge distribution at the origin of the coordinates. In the MCDF model, an atomic state function (ASF) is represented as linear combination of configuration state functions (CSF) of the same parity ($P$) and total angular momentum ($J,M$)

$$|\psi_\alpha(PJM)\rangle = \sum_r^{n_c} c_r(\alpha)|\gamma_r PJM\rangle, \qquad (3)$$

and where $n_c$ is the number of CSFs and (the mixing coefficients) $\{c_r(\alpha)\}$ a representation for the atomic state within the given basis. In the GRASP92 program [32], the CSF are taken as antisymmetrized products of a common set of *orthonormal* orbitals which are optimized self-consistently based on the Dirac-Coulomb Hamiltonian

$$H_{\mathrm{DC}} = \sum_i h_D(\mathbf{r}_i) + \sum_{i>j} \frac{1}{r_{ij}}. \qquad (4)$$

In this Hamiltonian, the one-electron Dirac operator

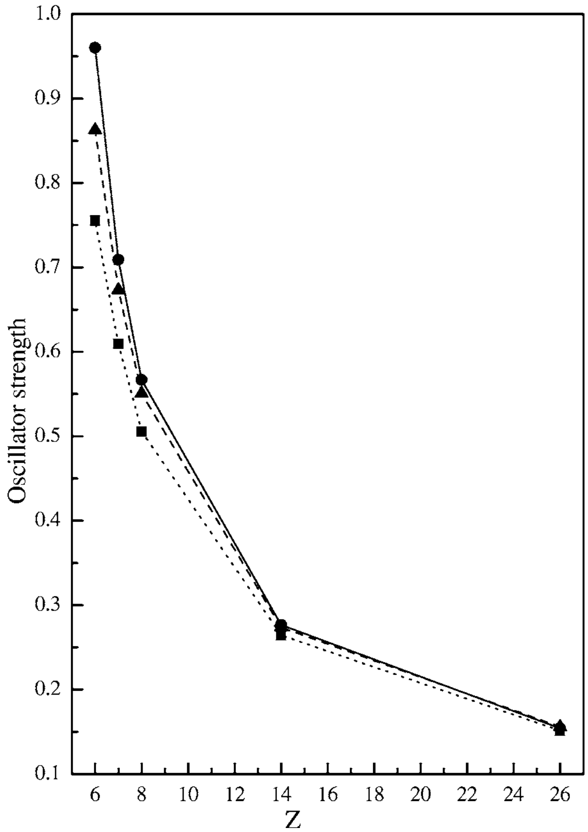


FIG. 3. Variation of oscillator strength of the $2s^2\,{}^1S_0 \to 2s2p\,{}^1P_1^o$ transition as function of the nuclear charge and for a screening parameter $\lambda = 0.30$ a.u. Oscillator strengths are shown for zero-plasma screening (dotted line) and are compared with those for screening only the electron-nucleus interaction (solid line) and for screening both the electron-nucleus and the electron-electron interaction (dashed line).

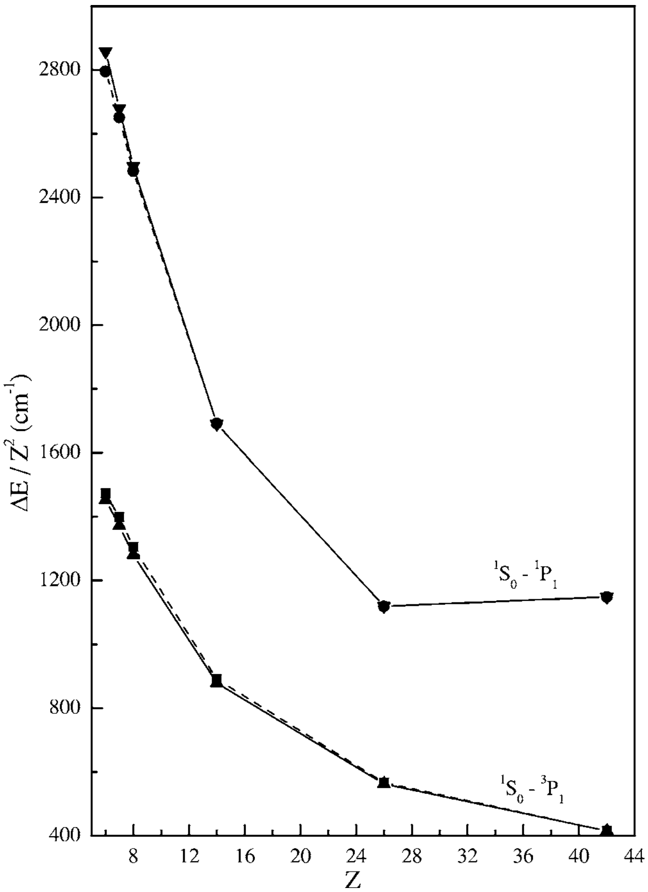


FIG. 4. Shift of the $2s^2\,{}^1S_0 \to 2s2p\,{}^1P_1^o$ and $2s^2\,{}^1S_0 \to 2s2p\,{}^3P_1^o$ transition energies (scaled by $Z^{-2}$) as function of the nuclear charge; calculations without screening (solid line) are compared with those for $\lambda = 0.20$ a.u., taking the screening into account for both the electron-nucleus and electron-electron interaction.

$$h_D = c\alpha \cdot \mathbf{p} + \beta \mathbf{c}^2 + \mathbf{V}(\mathbf{r}) \tag{5}$$

describes the kinetic energy of the electron and its interaction with nucleus and any mean field from the environment. For a Debye-Hückel plasma model, therefore, we may include the plasma screening effects directly into the MCDF equations. Combining Eqs. (1) and (5), the one-electron Dirac operator is given in the presence of plasma background by

$$h_D^{\mathrm{DH}} = c\alpha \cdot \mathbf{p} + \beta \mathbf{c}^2 + \mathbf{V}^{\mathrm{DH}}(\mathbf{r_i}, \lambda) \tag{6}$$

and, hence, the modified relativistic Dirac-Coulomb Hamiltonian in a Debye-Hückel plasma by

$$H_{\mathrm{DC}}^{\mathrm{DH}} = \sum_i h_D^{\mathrm{DH}}(\mathbf{r}_i, \lambda) + \sum_{i>j} V^{\mathrm{DH}}(r_{ij}, \lambda). \tag{7}$$

As known from any many-particle calculation, of course, the main effort concerns the evaluation (and computation) of the electron-electron interaction. To derive the modified two-particle integrals due to the plasma screening, we may write the second term on the right-hand side (rhs) of Eq. (7)

$$V^{\mathrm{DH}}(r_{ij}, \lambda) = -\lambda \sum_{l=0}^{\infty} (2l+1) j_l(i\lambda r_<) h_l^1(i\lambda r_>) P_l(\cos\theta) \tag{8}$$

in terms of the *larger* $[r_> = \max(r_i, r_j)]$ and *smaller* radii $[r_< = \min(r_i, r_j)]$ of the one-particle radii $r_i$ and $r_j$, respectively, and where $j_l$ denotes a Bessel function and $h_l^1$ a Hankel function of the first kind. While the incorporation of the screening into the electron-nucleus interaction usually destabilizes the binding of the electron, the screening of the electron-electron repulsion counteracts this trend. Many interesting features in the transition properties of multiple charged ions therefore arise from the *net* effect in screening the electron-nucleus *and* the electron-electron interaction, and how they affect the formation of the electron shells in the ion.

### III. COMPUTATION

The plasma model outlined above has been utilized in order to investigate the influence of the plasma screening upon the excitation energies and transition probabilities for the Be-like ions embedded in a *weakly coupled hot* plasma. For a moderate external field, the low-lying level structure of the Be-like ions consists of the even-parity $1s^2 2s^2\,{}^1S_0$ ground state as well as the four $1s^2 2s2p$ odd-parity excited levels with total angular momenta $J = 0, 1, 2$. From these excited

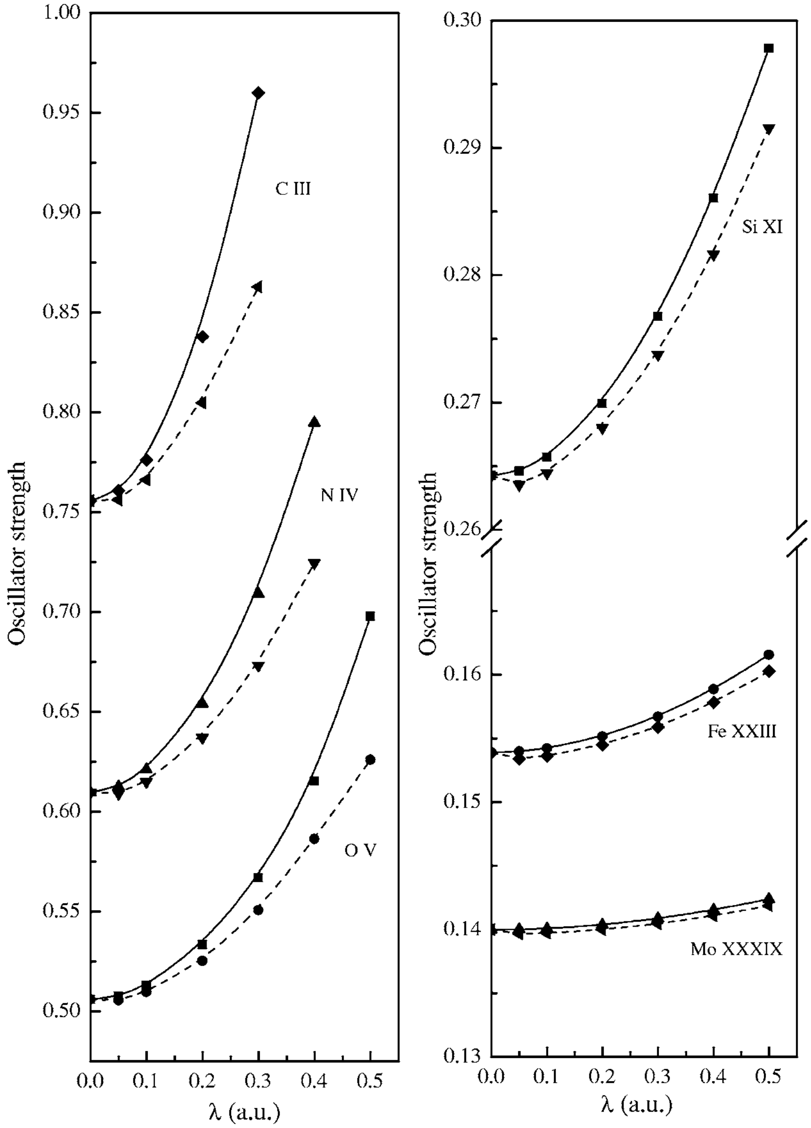


FIG. 5. Variation of the oscillator strength of the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1^o$ resonance transition as function of the plasma screening parameter $\lambda$. Results are compared from two computational models including the plasma screening for only the electron-nucleus interaction (solid line) and for both the electron-nucleus and electron-electron interaction (dashed line), respectively.

levels, only the two levels with $J=1$ can decay by allowed and intercombination (electric-dipole) transitions to the $^1S_0$ ground state.

Using the $2s^2$ and $2s2p$ reference configurations from above, we incorporated all single (S) and double (D) excitations from the $2s$ and $2p$ valence shells into the $nl$ ($n=3,4,5$) unoccupied shells, leaving the $1s^2$ core unaffected. In the computations of the wave functions for the C III and N IV ions, we included SD replacements of the valence electrons outside the $1s$ core up to the $5f$ subshells while, for all higher charges, these replacements were restricted to the $3l$ and $4l$ subshells. In this computational model, the wave function expansion (3) contains 2948 CSF for the C III and N IV ions and 1359 CSF for all others. For the isolated ions, this size of the wave function expansions allows us to reproduce the experimental excitation energy [34–36] within about 0.2% and 0.5% for the spin-forbidden and resonance transitions, respectively, and is thus sufficient in its accuracy for the present investigations. Having generated the wave functions for the Be-like ions, the transition properties have been calculated by means of the RATIP suite of programs [33].

## IV. RESULTS AND DISCUSSION

In the present paper, we explore and analyze the influence of the plasma screening on the Be-like C III, N IV, O V, Si XI, Fe XXIII, and Mo XXXIX ions in the framework of the MCDF model. Emphasis has been placed on the (electric) dipole-allowed $2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1^o$ and spin-forbidden $2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1^o$ transition between the low-lying levels of these ions. The intensity ratio of these two lines plays an important role in plasma diagnostics for determining the electron density of astrophysical sources, such as the Sun and the stellar corona or for terrestrial sources, including tokamaks.

In our computations below, the wave functions have been generated self-consistently for each value of the screening parameter $\lambda$, taking two models into account for the screening of the interatomic interactions: While (1) only the screening between the electron-nucleus interaction is considered, we include (2) both, the screening between the electron-nucleus and the electron-electron interactions. Transition properties, such as the excitation energies, oscillator strengths, or transition probabilities are calculated for a wide

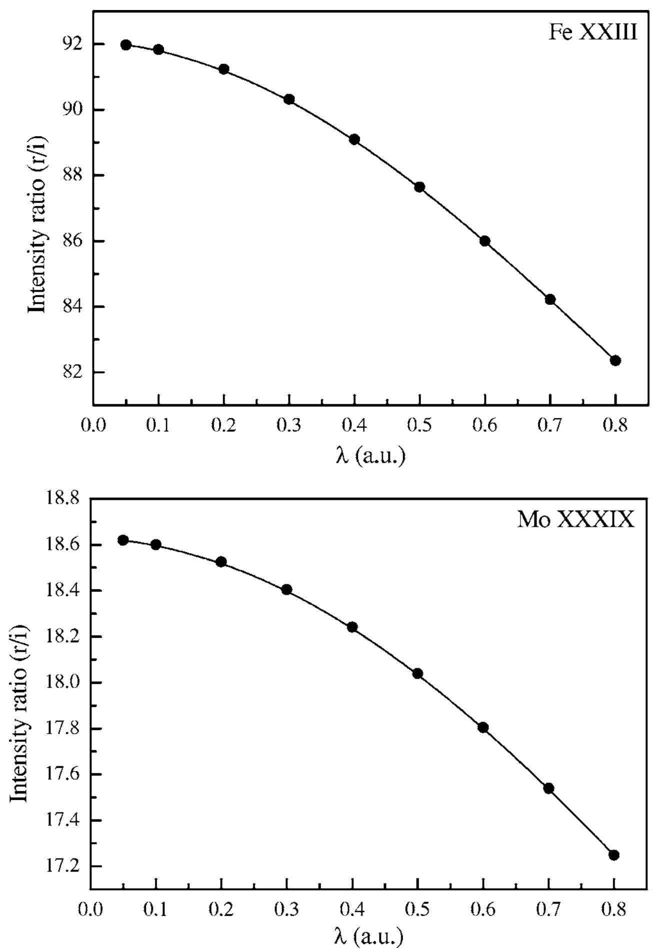


FIG. 6. Intensity ratio of the resonance ($r$) to the intercombination ($i$) line as function of the plasma screening parameter λ. Results are shown for the two ions Fe XXIII and Mo XXXIX.

range of screening parameters, e.g., for $\lambda=0.00$, 0.05, 0.10, 0.20, 0.30, 0.40, and 0.50 a.u. For these values of λ, the plasma-coupling parameter ($\Gamma=q^2/4\pi\epsilon_0 dkT$ for particles separated by a typical distance "$d$"), which describes the ratio of the electrostatic energy of neighboring particles and the thermal energy, is much smaller than unity, that is the statically shielded Debye-Hückel potential in Eq. (1) is appropriate to describe the screened Coulomb interaction [37].

Figure 1 displays the effect of the plasma screening on the excitation energy of the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^3P_1^o$ intercombination transition. For this spin-forbidden line, the transition energy increases rather rapidly for all ions along the beryllium isoelectronic sequence as the screening parameter is enlarged from $\lambda=0.00$ to 0.40 a.u. Since λ is proportional to the ratio $(n_e/T_e)^{1/2}$ [cf. Eq. (2)], this means that, for a given plasma temperature ($T_e$), the transition energies become more and more blueshifted as the plasma density increases. As seen from Fig. 1, however, the increase of the excitation energy of the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^3P_1^o$ intercombination line is mainly determined by the screening of the electron-nucleus interaction, while the plasma effects on the electron-electron interaction only play a minor role. In general, we find $|\Delta E_{ne+ee}| < |\Delta E_{ne}|$ for the $^1S_0 - ^3P_1^o$ intercombination transition for all ions along the Be sequence. As expected, moreover, the plasma screening becomes less important for higher nuclear charges $Z$, if taken relative to the wavelength of the free ions. For berylliumlike oxygen and silicon, for example, this blueshift amounts to 346 and 336 $\mathrm{cm}^{-1}$ for a screening parameter of $\lambda=0.10$ a.u. or, equivalently, to a relative shift of the transition energies of 0.45% and 0.18% for these ions, respectively.

Apart from the effects of the static screening above, the (so-called) "dynamic screening" has been found important for both weak and strongly coupled plasmas as discussed extensively in the literature [6,38–43]. In the present case, however, we may restrict ourselves to the limit of static screening as we explore low-density plasmas and rather high excitations of atomic levels. For such plasma conditions, we can safely assume $\epsilon(Q,\omega)\approx 1$ for $\omega_L^2/\omega^2 \ll 1$, where $\omega_L$ refers to the plasma frequency and $\hbar\omega$ denotes the excitation energy. Since the excitation energies of the $^{1,3}P_1$ levels are sufficiently large for all the Be-like ions, this condition is well fulfilled for plasma densities up to $10^{22}\ \mathrm{cm}^{-3}$ and if a plasma temperature of 1 keV is assumed. In the present work, therefore, these dynamical plasma polarization effects can be neglected throughout [17].

For the $2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1^o$ allowed transition, the effect of the plasma screening is seen from Fig. 2, showing a quite remarkable behavior for the different berylliumlike ions. For this "resonance line," the shift of the transition energy strongly depends on both the screening parameter λ and the nuclear charge $Z$ of the ions. Again, the inclusion of the plasma screening into the electron-electron interaction counteracts the shifts in the transition frequency as obtained for the case in which only the electron-nucleus would be screened. For berylliumlike nitrogen (N IV) and oxygen (O V), this inclusion of the plasma screening into the electron-electron repulsion may change even the sign of the shift as seen from Fig. 2. A similar behavior is expected also for the oscillator strength (cf. Fig. 3) as the electric-dipole operator is $\sim r$ and, hence, the oscillator strength is stronger influenced at large values of $r$ owing to the plasma corrections to the potential. With increasing $Z$, of course, all the bindings become stronger and the plasma screening effects less important for a given value of λ.

While the resonance line of the light ions C III and N IV ions is redshifted for all screening parameters (up to $\lambda=0.40$ a.u.), the sign of the line shifts depends on λ for the heavier ions Si XI, Fe XXIII, and Mo XXXIX, starting with a redshift for small values $\lambda \lesssim 0.20$ a.u. and leading to a blueshift as the screening parameter (λ) is increased. For $\lambda=0.10$ a.u., for instance, the redshifts are 693 and 3880 $\mathrm{cm}^{-1}$ for N IV and Mo XXXIX, respectively.

Figure 4, finally, shows the total shifts in the $^1S_0 - ^{1,3}P_1^o$ excitation energies as functions of the nuclear charge $Z$ and for fixed $\lambda=0.20$ a.u. This value of λ corresponds to an electron density of about $10^{21}\ \mathrm{cm}^{-3}$ for a temperature of 1 keV, which is typical in inertial fusion or for magnetic fusion reactors. Although the overall trend is similar for both the $^1S_0 - ^1P_1^o$ resonance and $^1S_0 - ^3P_1^o$ intercombination line, it is observed that in case of $^1S_0 - ^1P_1^o$ resonance line, the total shift changes from red to blue for high-$Z$ ions as λ increases.

The changes in the oscillator strengths as function of the plasma screening are summarized in Figs. 5 and 6. As seen from Fig. 5, for example, the oscillator strength of the $2s^2\,{}^1S_0 \rightarrow 2s2p\,{}^1P_1^o$ resonance transition increases as the screening or, equivalently, the electron density increases (for a given temperature of the plasma). Of course, the same trend is found also for the emission rate ($A$) of this line for all the ions under investigation. When compared to the resonance line, however, a larger shift is typically obtained for the ${}^1S_0 - {}^3P_1^o$ intercombination line, leading to clear decrease of the intensity ratio of the resonance to the intercombination line as function of the plasma parameter $\lambda$. For Fe XXIII and Mo XXXIX ions, we plotted (see Fig. 6) the resonance-to-intercombination line intensity ratio for the screening parameters $\lambda = 0.05, \ldots, 0.80$ a.u., the corresponding electron densities are between $10^{20}$ and $10^{22}$ cm$^{-3}$, assuming an electron temperature of 1 keV.

## V. CONCLUSIONS

In summary, we have investigated the effects of the plasma screening on the transition properties such as the excitation energies, oscillator strengths and transition probabilities of the Be-like ions. Multiconfiguration Dirac-Fock wave functions have been used to analyze the screening of the electron-nucleus and electron-electron interaction in hot and weakly coupled plasmas (Debye-Hückel model). Beside of the transition properties, we also report about the resonance-to-intercombination intensity ratio as function of the plasma screening. The intensity of transitions with very different rates, but originating from closely lying upper energy levels, can give information about the local electron density in a plasma [44]. Moreover, the relative line strengths of the Be-like ions in a high temperature plasma can be used in order to derive the electron temperature and density of the plasma in the emitting region through the diagnostics of the line ratios. The relative line intensities are presented graphically, so that they can be used easily by tokamak researchers. In general, the incorporation of the plasma screening into the electron-electron interaction counteracts the behavior of the energies and transition properties when compared to the case that only the screening of the electron-nucleus interaction is taken into account. In practice, however, the effects of plasma screening onto the resonance and intercombination lines is often quite different in nature. While only a blueshift is observed for the ${}^1S_0 - {}^3P_1^o$ intercombination transition for all elements along the Be sequence, the resonance line can be either blueshifted or redshifted in dependence on the screening parameter and the particular ion under investigation.

In the literature, a screened Coulomb potential has been applied by many authors in the past in order to obtain insight into the collective behavior of both laboratory and astrophysical plasmas [45], cf. Sec. I. However, since the screened potential is usually obtained by assuming the conditions of a thermodynamic equilibrium and, in particular, that the thermal energy is much larger than the potential energy (to make the linearization the Poisson equation), care should be taken in the interpretation of the corresponding results. In fact, it is now well established that the Debye-Hückel model can describe the plasma reliably only when the screening length, i.e., $\lambda_D = 1/\lambda$, is large enough so that the Debye sphere contains a sufficiently large number of electrons [46]. We therefore hope that the present work will provide useful information to the plasma physics and astrophysics researcher.

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