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the line broadening, the line shift and the disappearance of the line emission (corresponding to the ionization potential depres-

sion IPD of the upper level). The IPD is of great interest for

applications in thermodynamics and also for the understand-

ing of the various radiative properties (emission, absorption,

scattering). Since decades, the working horse in dense plasma

atomic physics has been a plasma screening potential that acts

as a perturber for the free atom Hamiltonian. The screening po-

tential is induced by the charged particle distribution around the

ions in plasmas and is rather complex as it involves microfield

fluctuations of correlated charged particles. Among a large va-

riety of approaches, the Debye model [18, 7, 19], the Ecker-

Kröll model [20], the ion sphere model [21, 7], the Stewart-

Pyatt model [22], the Atomic-Solid-Plasma model [23] and the

Thomas-Fermi model [24, 25, 26, 7] have widely been applied

self-consistent finite temperature ion sphere SCFTIS model: it

Of particular interest in dense plasma atomic physics is the

and made important contributions in the field.

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### Analytical approach to level delocalization and line shifts in finite temperature dense plasmas

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#### Abstract

X-ray line shifts and delocalization of levels of He-like ions are studied within the framework of the self-consistent multi-configuration relativistic finite temperature ion sphere model. A set of analytical equations for an N-electron bound atomic system to determine X-ray line shifts and level delocalization is proposed that provides very good agreement with numerical calculations, newly high precision line shift measurements of the 1s3p  $^{1}P_{1}-1s^{2}$   $^{1}S_{0}$   $He_{\beta}$  transition in  $Cl^{15^{+}}$  and the 1s3p  $^{1}P_{1}$ -level delocalization in  $Al^{11^{+}}$ . We re-analyzed the recently claimed discrepancy between the predictions from the ion sphere model, analytical approaches and the data. The analytical b-potential approach that imitates lattice effects via a perturbation of the free electron distribution in the in sphere is developed and contrasted with currently unexplained line shift measurements of the  $1s2p {}^{1}P_{1} - 1s^{2} {}^{1}S_{0} He_{\alpha}$  transition in  $Al^{11^{+}}$ .

Keywords: Atomic structure, ionization potential depression, finite temperature ion sphere model, laser produced plasmas, X-ray spectroscopy

#### 1. Introduction

The atomic populations are the fundamental quantity for various different disciplines in science and applications, like e.g. the equation of state in thermodynamics, absorption, emission and scattering properties of matter, lasing, radiation transport, radiative cooling and energy loss, diagnostic and spectroscopy employing the radiative properties of matter, astrophysics, planetary science, radiation sources, fusion science [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. In a low-density environment, where atoms and ions are essentially free, atomic population kinetics of gases and plasmas has been very successful in many different scientific and technical disciplines. As density increases, the free atom model breaks down resulting in a perturbation of the atomic energy levels. The perturbation of atomic levels manifests itself essentially in a broadening and a shift. These perturbations can be observed in high-resolution spectroscopic experiments via the analysis of

allows to combine dense plasma effects in a very general manner [7] with the numerical solution of the Schrödinger or Dirac 1 © 2020 published by Elsevier. This manuscript is made available under the CC BY NC user license

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equation and allows reaching spectroscopic precision. It is therefore well suited to compare simulations with the data that are obtained in the overwhelming number of cases by spectroscopic methods. Recent measurements have questioned our understanding in the precision of the Multi-Configuration-Dirac-Fock Self-Consistent Finite Temperature Ion Sphere model MCDF-SCFTIS [7, 27, 28]: it was claimed [29] that measured line shift values are significantly smaller than predictions from the selfconsistent-field ion-sphere model. However, later numerical analysis showed [30, 31, 32, 33] that excellent agreement with the finite temperature ion sphere model, the arbitrary perturbation potential method APPM [34], the analytical b-parameter potential method [32] and the data is obtained.

In this letter we report on a critical analysis of recent highresolution spectroscopic data on X-ray line shift measurements [29] and analytical approximations of numerical solutions. We develop a 4<sup>th</sup>-order analytical approximation of the arbitrary perturbation potential method APPM [34] and demonstrate excellent agreement with the present MCDF - SCFTIS calculations and the data. The analytical approach is generalized for an Nbound-electron system and its total energy shift that is expressed in terms of electron temperature, electron density, principal and orbital quantum number of core bound and optical electrons (described with scaled H-like matrix elements). This analytical approach has spectroscopic precision and is successfully applied to the analysis of line shifts and orbital delocalizations. Its simplicity allows implementation in complex integrated simulations in high energy density physics.

Finally, we develop an analytical solution of an N-electron bound system for the b-parameter potential proposed recently [32] and discuss the results with currently unexplained line shift measurements of the  $1s2p^{1}P_{1}-1s^{2} {}^{1}S_{0}$   $He_{\alpha}$  transition in  $Al^{11^{+}}$  [35].

# 2. X-ray spectroscopic data versus Self-Consistent Finite Temperature Ion Sphere model

The Multi-Configuration-Dirac-Fock Self-Consistent Finite Temperature Ion Sphere model assumes that the dense plasma is composed of ion spheres and solves self-consistently the Nbound electron Dirac-Hamiltonian together with the Poisson equation determined by the free electron plasma density  $n_f(r)$ and the bound electron density  $n_b(r)$  inside the ion sphere and the nuclear charge  $Z_n$ . Each ion-sphere contains one nucleus at the center and numbers  $N_f$  and  $N_b$  of free and bound electrons, respectively to keep the ion sphere neutral, i.e.  $Z_n - N_f - N_b = 0$ or equivalent  $Z_n - N_b = \frac{4\pi}{3}R^3n_e$ , where R is the ion sphere radius and  $n_e$  is the average plasma free electron density in the ion sphere. The bound electron density is given by

$$n_b(r) = \frac{1}{4\pi} \sum_{j=1}^N q_j \left[ P_j^2(r) + Q_j^2(r) \right].$$
(1)

where N is the number of bound electrons,  $q_j$  is the number of electrons in the subshell j, and  $P_j(r)$  and  $Q_j(r)$  are the radial wave functions of the large and small components of orbit j, respectively. More details are described in [7, 27, 28, 36].



Figure 1.  $He_{\beta}$  and  $He_{\alpha}$  line shifts for different ions and electron temperatures and fixed electron density  $n_e = 3 \times 10^{23} cm^{-3}$  obtained from the present MCDF-SCFTIS calculations. Also shown are the ratios between the  $He_{\beta}$  and  $He_{\alpha}$ line shifts and the Z-scaled line shifts of  $He_{\beta}$  (multiplied by 1/16 for better demonstration).

The solid curves in Fig. 1 represent the theoretical line shifts of  $He_{\beta}$  and  $He_{\alpha}$  for different atomic number of He-like ions obtained from the present MCDF-SCFTIS calculations,  $n_e$  =  $3 \times 10^{23} cm^{-3}$ . It can be seen, that the line shift of the  $He_{\beta}$ -line is about 5 times larger than those of the  $He_{\alpha}$ -line. Also shown are the ratios of these line shifts (dashed lines): a very weak dependence on atomic number is observed for various electron temperatures. The bold solid blue and red lines (designated as "Z-scaled" in Fig. 1) present the  $He_{\beta}$ -line shifts for different temperatures in a Z-scaled representation, i.e.  $\Delta E_{He\beta} \times (Z_n - N_b)$ (note, that for better demonstration in the same figure the scaled results have been divided by a factor of 16). It can likewise be seen, that the dependence on atomic number is also very weak for the scaled shifts. The weak Z-dependence of the scaled shifts is related to parameter cases of hot dense plasmas where the first two positive terms in the APPM [34] are dominant over the negative terms. Numerical calculations for different densities and temperatures indicate similar weak dependences. A comparison of the measured line shifts of the  $He_{\beta}$  line for a suitable atomic element and different plasma parameters constitutes therefore a relevant test for the MCDF-SCFTIS model that is considered below.

Figure 2 compares the present MCDF-SCFTIS model calculations (red and green crosses, connected with dashed lines) with the measurements (open and solid circles) of the  $He_\beta$  line shifts of  $Cl^{15^+}$  of [29]. As can be seen the present MCDF-SCFTIS calculations are in excellent agreement with the measurements. Also indicated in the figure are the results from the average ion sphere model [30] (pink solid circles connected with solid line) that provide systematically higher line shift values. Note, that the average atom ISM does not include multi configuration and intermediate coupling effects as does the present MCDF-SCFTIS model, more details are described in [28]. Within the large experimental error bars, we can therefore confirm the



Figure 2. Comparison of the present MCDF-SCFTIS calculations (red and green crosses, connected with dashed lines) for the line shift of the  $He_{\beta}$  line of  $Cl^{15+}$ , the present analytical model (solid black square, connected with dashed line) and the spectroscopic data (open and solid black circles) of [29]. Also shown in the figure our present results employing the analytical model of [36] ( $4^{th}$ -order blue crosses,  $2^{nd}$ -order solid blue and red lines) and the average atom ion sphere model ISM from [30] (pink solid circles, connected with solid line).

statements made in [30, 33] that the measured red shifts show very good agreement with the predictions of the finite temperature ion sphere model.

Let us now shed more light into the various analytical approximations. Based on the APPM [34] an analytical potential for the electron free energy at finite temperature has been derived in the framework of the ion sphere model at finite temperature. This potential has then been expressed in terms of reduced matrix elements  $(x^{3/2})$  [34] that does have an analytical representation that is simple and of closed form (it can only be expressed in terms of non-integer Gamma functions [37]). In the work [36] a 2<sup>nd</sup>-order analytical approximation has been developed that is expressed in terms of simple analytical H-like dipole and quadrupole matrix elements of closed form. Figure 2 shows also the line shifts obtained from this 2<sup>nd</sup>-order analytical approximation (blue solid and red solid, designated as "Li-Rosmej  $2^{nd}$ -order" in the figure): they are systematically too large compared with the data. The curves with blue crosses (indicated as "Li-Rosmej 4<sup>th</sup>-order" in Fig. 2) show the results when developing the analytical approach of [36] up to the 4<sup>th</sup>-order in terms of simple analytic, closed form H-like matrix elements. It can be seen, that the 4<sup>th</sup>-order analytical approach of [36] provides excellent agreement with the data and also with the numerical calculations. Therefore the differences between the analytical approach of [36] and the data of [29] turn out not to be a conceptual deficiency in the finite temperature ion sphere theory as discussed in [29] but rather to be an effect of the limited precision of the 2<sup>th</sup>-order approximation of the present MCDF-SCFTIS model compared to the 4<sup>th</sup>-order series expansion (more details are given in the appendix).



Figure 3. Relative changes of the spontaneous transition probabilities of  $He_{\alpha}$  and  $He_{\beta}$  of  $Cl^{15+}$  calculated from the present MCDF-SCFTIS model for different densities and temperatures.

In a dense plasma environment, not only the energy level shift but also the spontaneous transition probabilities are affected. As almost all experimental data for line shifts are obtained by spectroscopic measurements of line intensities in dependence of the frequency, possible perturbation of the Einstein spontaneous transition probabilities A due to the dense plasma environment are also of interest. Fig. 3 shows the relative changes of the transition probabilities as obtained from the present MCDF-SCFTIS model. It can easily be seen, that the relative changes for the  $He_{\alpha}$ -line of  $Cl^{15+}$  are not important for the present analysis: much below one percent even for near solid densities. Likewise, also the  $He_{\beta}$ -line is only affected up to a few percent. Therefore, changes in transition probabilities due to dense plasma effects are negligible for the present analysis and discussion of X-ray line shifts of the He-like  $Cl^{15+}$  ions in hot near solid density plasmas.

Let us now apply the MCDF-SCFTIS model to the study of the 1s3p <sup>1</sup> $P_1$ -level delocalization in  $Al^{11^+}$  as measured in [38]: At  $n_e = 2.0 - 2.5 \times 10^{24} cm^{-3}$  and  $kT_e = 700 eV$  the  $He_{\beta}$ -line of  $Al^{11+}$  is not observed, while at  $n_e = 8.6 - 11 \times 10^{23} cm^{-3}$  and  $kT_e = 700eV$  the  $He_{\beta}$ -line is clearly observed. For these parameters, the present MCDF-SCFTIS model calculations provide ionization potential depression values of 196eV - 205eVand 158eV - 169eV, respectively. The analytical model of [36] in  $4^{th}$ -order expansion (see also appendix) provides 198eV – 210eV and 157eV - 169eV, respectively and is therefore in very good agreement with the numerical calculations of level delocalizations too. Because the free atom ionization potential of the 1s3p  $^{1}P_{1}$ -level is 220eV (as calculated from our MCDF-SCFTIS model) we conclude that  $He_{\beta}$  should not be observed if the ionization potential depression IPD reaches the value of the free atom ionization potential. As the  $\beta$ -line widths due to the Stark effect are of the order of 50eV (Stark broadening calculations show that the FWHM of  $He_{\beta}$  at 300eV and  $n_e = 1 \times 10^{23} cm^{-3}$  is about 15 eV while at  $n_e = 1 \times 10^{24} cm^{-3}$  the

FMHM is about 60eV), the  $He_{\beta}$ -line should not be observed for the highest densities while for the lower ones  $He_{\beta}$  should be observed. This is in rather good agreement with the experimental observations.

#### 3. Analytical formulas for the total energy shift of an Nbound electron system

Self-consistent numerical calculations of the MCDF and the Poisson equations are not very convenient neither for dense plasma atomic physics studies nor for integrated simulations in high-energy density physics. We therefore develop a set of analytical closed form equations for a perturbation potential in atomic physics calculations that has spectroscopic precision (line shifts) and allows precision predictions of level delocalization. For these purposes we employ a free electron plasma screening potential of the form [32]

$$\phi_f(r) \approx \frac{N_f}{R} \left[ 1 + \frac{1}{x-1} - \frac{1}{x-1} \left( \frac{r}{R} \right)^{x-1} \right],$$
 (2)

where

$$x = 3 - \frac{b \cdot e}{\pi} \sqrt{\frac{N_f}{RT_e}} \tag{3}$$

where R is the ion sphere radius. The free electron distribution  $P_f(r)$  is assumed to have the functional dependence according

$$P_f(r) = \frac{N_f}{R^x} \cdot r^x \tag{4}$$

that is consistent with the limit of the Uniform Electron Gas Model UEGM where x = 3. b is a parameter that characterizes the self-consistent electron distribution in the ion sphere, e.g. for a Maxwellian electron distribution the MCDF-SCFTIS simulations are matched with  $b \approx 2$ , while IPD values of near solid density matter could be described with  $b \approx 4$  [32]. We note, that approximation (3) is of very good quality if  $N_f e^2 \leq RT_e$ .

Employing first order perturbation theory we find for the energy shift of the N-electron system

$$E_{p} = \left\langle \Psi_{0}(r_{1}, ..., r_{N}) \left| \sum_{i=1}^{N} \phi_{f}(r_{i}) \right| \Psi_{0}(r_{1}, ..., r_{N}) \right\rangle$$
$$= \sum_{i=1}^{N} \frac{N_{f}}{R} \left[ 1 + \frac{1}{x-1} - \frac{1}{x-1} \frac{1}{R^{x-1}} \left\langle r_{i}^{x-1} \right\rangle \right], \tag{5}$$

where  $\langle r_i^{x-1} \rangle$  is the mean value of  $r^{x-1}$  for the *i*<sup>th</sup> bound electron.  $E_p$  can be calculated analytically if  $\langle r_i^{x-1} \rangle$  has an analytical solution. For H-like ions  $\langle r^{\beta} \rangle$  can be expressed by the Gamma function  $\Gamma$  for any real  $\beta$  [37]:

$$\left\langle n,l\left|r^{\beta}\right|n,l\right\rangle = (-1)^{n-l-1} \left(\frac{n}{2\cdot Z}\right)^{\beta} \frac{1}{2n} \times \sum_{i=0}^{n-l-1} \frac{\zeta(i) \times \Gamma(2l+3+i+\beta)\Gamma(2+i+\beta)}{\Gamma(2l+2+i)\Gamma(n-l-i)\Gamma(l+3-n+i+\beta)},$$
(6)

$$\zeta(i) = \frac{(-1)^i}{\Gamma(i+1)},\qquad(7)$$

where  $\beta = x - 1$  and  $Z = Z^{eff}$  (if the hydrogen-like approach is used for the *N* bound-electron system). The Gamma-function itself has no analytical closed form solution but can easily be evaluated, e.g. with the method of P. Godfrey [39]. Therefore, the total energy shift for the *N* bound-electron system can approximated by the expression

$$E_p = \sum_{i=1}^{N} \frac{N_f}{R} \left[ 1 + \frac{1}{x-1} - \frac{1}{x-1} \frac{1}{R^{x-1}} \left\langle r_i^{x-1} \right\rangle \right], \tag{8}$$

where

$$\left\langle r_{i}^{x-1} \right\rangle = (-1)^{n-l-1} \left( \frac{n}{2 \cdot Z_{i}^{eff}} \right)^{x-1} \frac{1}{2n} \times \sum_{i=0}^{n-l-1} \frac{\zeta(i) \times \Gamma(2l+3+i+x-1)\Gamma(2+i+x-1)}{\Gamma(2l+2+i)\Gamma(n-l-i)\Gamma(l+3-n+i+x-1)}.$$
 (9)

 $Z_i^{eff}$  is the effective nuclear charge for the *i*<sup>th</sup> bound electron and (n, l) are the principle and angular quantum numbers of the *i*<sup>th</sup> bound electron. The effective nuclear charge can be calculated by  $Z_i^{eff} = n \sqrt{2E_i}$ , where  $E_i$  is the energy of the *i*<sup>th</sup> bound electron. If only one electron is involved in the atomic transition, the corresponding spectral shift  $\Delta E_{shift}$  can be easily calculated by the difference of the energy shift between the two orbits *i* and *j* involved, i.e.

$$\Delta E_{shift} = \left| \frac{N_f}{x - 1} \frac{1}{R^x} \left( \left\langle r_j^{x - 1} \right\rangle - \left\langle r_i^{x - 1} \right\rangle \right) \right| \tag{10}$$

Fig. 2 presents also the analytical approximation of Eq. (10) (solid black squares, connected with dashed line, b = 2) that demonstrates very good agreement with the numerical calculations and the data.

Concerning the 1s3p  ${}^{1}P_{1}$ -level delocalization in  $Al^{11^{+}}$  at  $n_{e} = 2.0 - 2.5 \times 10^{24} cm^{-3}$ ,  $kT_{e} = 700eV$  and  $n_{e} = 8.6 - 11 \times 10^{23} cm^{-3}$ ,  $kT_{e} = 700eV$  we obtain (with b = 2) 201eV - 212eV and 159eV - 171eV, respectively being in very good agreement with the numerical calculations. This proofs that the analytical potential of eq. (2) has a good spectroscopic precision and therefore considerably facilitates dense plasma atomic structure calculations (because no self-consistent approach with the Poisson equation has to be invoked).

#### 4. Discussion of the analytical b4-potential

Figure 4 shows the line shift measurements of the  $1s2p {}^{1}P_{1}-1s^{2} {}^{1}S_{0}$   $He_{\alpha}$  transition in  $Al^{11^{+}}$  [35]. It can clearly be seen, that the MCDF-SCFTIS simulations show much too small values up to a factor of 2.5 for the highest densities measured. The same holds true for the 4<sup>th</sup>-order analytical expression as well as for the analytical potential method with b = 2 that are very close to the MCDF-SCFTIS simulations. Also indicated in the figure are the results from the average ion sphere model [40] (pink solid circles, connected with solid line) that likewise show systematically much to small values compared to the measurements. Therefore, the line shift measurements of the  $1s2p {}^{1}P_{1} - 1s^{2} {}^{1}S_{0} He_{\alpha}$  transition in  $Al^{11^{+}}$  [35] remained unexplained up to present days.

It has been, however, demonstrated by [32] that the analytical potential of Eq. (2) with b=4 allows to match well the ionization potential measurements of solid density aluminum performed by femtosecond XFEL irradiation of the solid sample as does the Atomic-Solid-Plasma ASP model [23], while MCDF-SCFTIS simulations, the b2-potential (i.e. Eq. (2) with b = 2), the Ecker-Kröll model [20] (for discussion of the original and modified Ecker-Kröll model and its confusion in the literature see [23]), and the Stewart-Pyatt model [22] failed. These observations suggests, to use the b4-potential (i.e. Eq. (2) with b = 4) to investigate the line shift measurements of [35] that have also been performed near solid densities. The blue dots (connected with blue line) in Fig. 4 show the corresponding b4-potential line shift predictions while the blue dashed line includes the apparent line shifts of [35] (note that the apparent shifts have been defined as shift contributions other than plasma potential shifts, e.g. overlapping satellite contributions, for further discussion see [35]). The figure demonstrates excellent agreement of the b4-potential simulations with the data.

Could Fermi-Dirac effects in the free electron distribution be important ? This is unlikely, because the Fermi energy for the highest densities shown in Fig. 4 is  $\epsilon_F \approx 23eV$  while the electron temperature is  $kT_e \approx 300eV$ , i.e.  $\epsilon_F \ll kT_e$ . Therefore the chemical potential is close to its asymptotic Maxwellian value of  $\mu = -1.5 \cdot kT_e \cdot ln[(m_ekT_e/2\pi\hbar^2n_e^{2/3}]]$ . It is therefore suspected that the b4-potential might "imitate" lattice effects for the ionization potential depression and line shifts but a rigorous justification is still missing. We also note that line shift measurements of  $He_{\alpha}$  are rather complex for the reasons discussed in [23] and it appears helpful in view of the present discussion to have line shift measurements like those of [35] available for different low-Z-elements like, e.g. Na, Mg and Si.

#### 5. Conclusion

We have demonstrated that Multi-Configuration-Dirac-Fock Self-Consistent-Finite-Temperature-Ion-Sphere model calculations (MCDF-SCFTIS) and their analytical approximations are in excellent agreement with the data. Recent claims [29] of significant discrepancies between the line shifts of 1s3p  $^{1}P_{1} 1s^{2}$   $^{1}S_{0}$   $He_{\beta}$  in  $Cl^{15^{+}}$  and the analytical  $2^{nd}$ -order approximation of the ion sphere theory turned out not to be a conceptual deficiency in the ion sphere theory but rather to be an effect of the limited precision of the  $2^{nd}$ -order compared to the  $4^{th}$ -order series expansion.

Based on an analytical free plasma electron screening potential we derived a general analytical closed form expression (the "b-potential") for the ionization potential depression and line shift of an N-electron bound atomic system that is expressed only in terms of electron density, electron temperature, energies, principal and orbital quantum numbers. Comparisons with numerical calculations demonstrate very good agreement with the analytical N-electron approach over a wide range of plasma parameters. Finally, we discussed perturbations of the free electron distribution in the ion sphere by means of the analytical bpotential method. It was demonstrated, that the MCDF-SCFTIS simulations are well matched by  $b \approx 2$  while lattice effects are



Figure 4. Experimental  $He_{\alpha}$  line shift measurements of  $Al^{11+}$  [35] for different densities and their comparisons with different models. The analytic b4-potential provides a good agreement with the data. The dashed blue line shows the b4-potential data that include the apparent shifts [35] and excellent agreement with the measurements is observed. Also shown are the results from the average atom ion sphere model ISM from [40] (pink solid circles). Numerical calculations are carried out for  $kT_e = 250eV$ .

imitated with  $b \approx 4$ . We demonstrated, that the b4-potential matches well the line shift measurements  $1s2p \ ^1P_1 - 1s^2 \ ^1S_0$  $He_{\alpha}$  in  $Al^{11^+}$  of [35] that remained unexplained until present days. To what extent the analytical b-potential could imitate lattice effects for b > 2 remains an open question.

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#### Appendix A. Analytical 4<sup>th</sup>-order line shift and level delocalization formulas for finite temperature dense plasmas

Below, we provide explicit formulas for the analytical approach proposed in [36] (originally expressed in terms of simple analytical, closed form H-like dipole and quadrupole matrix elements) but in 4<sup>th</sup>-order approximation:

$$\Delta E_{nl} \approx 2Ry \cdot \frac{Z}{R_0} \cdot \frac{F\left(\left\langle r_i^1 \right\rangle, \left\langle r_i^2 \right\rangle, \left\langle r_i^3 \right\rangle, \left\langle r_i^4 \right\rangle\right)}{F\left(R_0, R_0^2, R_0^3, R_0^4\right)}$$
(A.1)

$$F(x_1, x_2, x_3, x_4) = \frac{R_0^2}{2} - \frac{x_2}{6} + \frac{4}{3\sqrt{\pi}} \cdot \sqrt{\frac{2RyZ}{kT_e}}$$

$$\times \left( R_0^{3/2} - \frac{2}{5} \left[ a_1 x_1 + a_2 x_2 + a_3 x_3 + a_4 x_4 \right] \right).$$
 (A.2)

 $Z = Z_n - N_b$  and the sum extends over the number  $N_b$  of bound electrons. It should be noted that the representation of the F-function in terms of expectation values  $\langle r_i^k \rangle$ , where k = 1, 2, 3, ... is just a convenient way because the integer matrix elements have analytical solutions that are simple, of closed form and only a few matrix elements are requested to achieve good approximations in relevant parameter intervals:

$$\langle r_i \rangle = \frac{1}{2Z_{eff}} \left[ 3n^2 - l(l+1) \right],$$
 (A.3)

$$\left\langle r_{i}^{2} \right\rangle = \frac{n^{2}}{2Z_{eff}^{2}} \left[ 5n^{2} + 1 - 3l(l+1) \right],$$
 (A.4)

$$\left\langle r_{i}^{3} \right\rangle = \frac{n^{2}}{8Z_{eff}^{3}} \left[ 35n^{2}(n^{2}-1) - 30n^{2}(l+2)(l-1) \right]$$
(A.5)

$$+ 3(l+2)(l+1)l(l-1)],$$
 (A.6)

$$\left\langle r_{i}^{4} \right\rangle = \frac{n^{4}}{8Z_{eff}^{4}} \left[ 63n^{4} - 35n^{2}(2l^{2} + 2l - 3) \right]$$
 (A.7)

$$+5l(l+1)(3l^{2}+3l-10)+12], \qquad (A.8)$$

$$Z_{eff} = n \sqrt{E_{nl}/Ry},\tag{A.9}$$

$$R_0 = 1.1723 \times 10^8 \left( Z/n_i \left< Z \right> \right)^{1/3}.$$
 (A.10)

Ry = 13.606eV,  $\Delta E_{nl}$  is the ionization potential depression energy in (eV),  $E_{nl}$  is the ionization potential (eV) of the optical electron with principal/orbital quantum numbers nl that move into an effective Coulomb potential with charge  $Z_{eff}$ ,  $Z_n$  is the nuclear charge,  $Z = Z_n - N_b$  where  $N_b$  is the number of bound electrons,  $n_i$  is the ion density in  $(cm^{-3})$ ,  $R_0$  is the corresponding averaged ion sphere radius in atomic units,  $\langle Z \rangle$  is the average charge of the plasma and  $kT_e$  is the electron temperature in (eV),  $a_1 = 0.77383$ ,  $a_2 = 0.36112$ ,  $a_3 = -0.01605$ ,  $a_4 = 0.000385182$ .

#### Appendix B. Numerical application for He-like argon

Let us apply the set of 4<sup>th</sup>-order analytical formulas for  $kT_e = 600eV$ ,  $n_e = 5 \times 10^{23} cm^{-3}$ ,  $Z_n = 17$ , Z = 15,  $\langle Z \rangle = 15$ ,  $E_{3p} = 386$ , 7eV,  $E_{1s} = 3658eV$ :  $\Delta E_{3p} = 169.44eV$ ,  $\Delta E_{1s} = 174.35eV$  and for the  $He_{\beta}$ -line shift of  $Cl^{15+} \Delta E_{1s-3p} = 4.9eV$  being in excellent agreement with the data presented in Fig. 2.

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