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Effect of dense plasmas on exchange-energy shifts in highly charged ions: An alternative approach for arbitrary perturbation potentials

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An alternative method of calculation of dense plasma effects on exchange-energy shifts ΔE_x of highly charged ions is proposed which results in closed expressions for any plasma or perturbation potential. The method is based on a perturbation theory expansion for the inner atomic potential produced by charged plasma particles employing the Coulomb Green function method. This approach allows us to obtain analytic expressions and scaling laws with respect to the electron temperature T, density n_e, and nuclear charge Z. To demonstrate the power of the present method, two specific models were considered in detail: the ion sphere model (ISM) and the Debye screening model (DSM). We demonstrate that analytical expressions can be obtained even for the finite temperature ISM. Calculations have been carried out for the singlet $1s2p\,^1P_1$ and triplet $1s2p\,^3P_1$ configurations of He-like ions with charge Z that can be observed in dense plasmas via the He-like resonance and intercombination lines. Finally we discuss recently available purely numerical calculations and experimental data.

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I. INTRODUCTION

Spectroscopic methods provide essential information about basic plasma parameters and relevant physical processes [1]. The accessible parameter range covers orders of magnitude in temperature and especially in density, because practically all elements of particular selected isoelectronic sequences can be used for diagnostic investigations. These elements may occur as intrinsic impurities or may be intentionally injected in small amounts (so called "tracer" elements). Apart from usual resonance line emission, the x-ray emission of dielectronic satellites is of great interest as they allow studying nonequilibrium phenomena [2] that become of increasing importance due to the rapid developments in short pulse laser technology (optical and free electron XUV/x-ray lasers), the fusion science, and high energy density physics.

Despite theoretical and experimental progress achieved in understanding dense plasma effects on atomic physics and on the spectral emission, this subject remains a controversy as it turns out to be extremely difficult to describe the excess of the free electrons around the ionic radiator which results in a perturbation of the bound electron energy levels and wave functions. The structure variations of the emitter energy levels therefore play a crucial role in the final radiation emitted from the plasma and the question "Which perturbation potential has to be used in the wave equations" is a central one: the relaxation of bound energy levels, the cutoff of principal quantum numbers, and the change of spontaneous transition probability, broadening, and shift of spectral lines have been known as characteristic dense plasma effects on emitting ions. X-ray spectroscopy of line transitions (to minimize absorption) therefore plays a key role in advancing the subject.

Apart from the usual observation of the Rydberg series of x-ray lines for Stark broadening analysis (including line shifts), the observation of intensities of resonance ($W = 1s\,2p\,^1P_1 \rightarrow 1s^2\ ^1S_0$) and intercombination ($Y = 1s\,2p\,^3P_1 \rightarrow 1s^2\ ^1S_0$) lines of highly charged ions is another effective diagnostic method due to (1) good signal to noise ratio, (2) resonance and intercombination lines (different spin states) are well separated from each other allowing their distinct observation even in dense plasmas despite of Doppler and Stark broadening, (3) opacity effects can be estimated directly from the emission spectra due to the low oscillator strength of the intercombination line, and (4) overlapping higher order satellite emission can be recalculated from the spectrally resolved $1s\,2l\,nl'$-satellite emission as all satellite series emission ($1s\,2l\,nl' \rightarrow 1s^2 2l + h\nu_{\mathrm{sat}}$) have the same dielectronic capture channel ($1s^2 + e \rightarrow 1s\,2l\,nl'$).

It has been proposed [3] that the energy difference between triplet $1s\,2p^3P_1$ and singlet $1s\,2p^1P_1$ states of helium-like aluminum (this difference being the double of the exchange energy between bound electrons) can be sensitive to the dense plasma environment. The theory [3] was based on direct self-consistent solution of multiconfiguration Dirac-Fock (MCDF) and Poisson equations for the radiating atom in a dense plasma providing entirely numerical results. The plasma environment was modeled in the ion-sphere model and a linear relation between the exchange-energy shift and electron density has been revealed. Relative line shift measurements [4] of the resonance and intercombination lines in dense laser produced plasma confirmed the hypothesis of dense plasma effects on the exchange-energy shift, however, the quantitative agreement with the data was poor.

It should be noted that there have been published a series of papers [5–12] devoted to calculations of plasma effects on atomic spectra mostly employing the Debye potential or its generalization. They provide a high precision of calculations from the atomic physics point of view (using correlated atomic state functions, variation principles, etc.) employing only a specific type of plasma-atom potential. However, neither the use of the Debye potential nor the use of Debye screened wave functions are rigorously justified nor a self-consistent approach involving the Poission equation (like those of Ref. [3]) was employed. From a physical point of view, the high precision is therefore inconsistent with the much less precise assumptions for specific plasmas potentials or screened wave functions.

In contrast to these approaches we try to develop a calculation method which can be applicable for every kind of plasma-atom potential in order to facilitate validation of different potentials by experimental data. The present method is based on a perturbation theory: the plasma-atom interaction is small as compared with strong Coulomb interaction inside the highly charge ions with nuclear charge $Z \gg 1$. The method can therefore be considered as a kind of (Z^{-1}) expansion which is well known as a very effective and precise method in atomic spectra calculations.

Moreover, the proposed method is essentially analytical and therefore allows extracting general scaling laws (meaning the general dependencies on atomic and plasma parameters) for every type of atom-plasma interaction. Detailed analysis is worked out for Debye and ion sphere models and a comparison with self-consistent numerical data [3] is presented.

For helium-like ions with high nuclear charge $(Z > 10)$, the nucleus-electron Coulomb interaction is predominant compared to any other interaction such as electron-electron interaction, plasma-electron interaction, etc. These interactions can be considered as perturbations compared to the Coulomb one and the Green function method is a suitable tool to treat this problem. Analytical expression for the Green function kernel has been given in terms of Coulomb wave functions [13,14]. This Green function method enables us to calculate the wave function variation when any small potential compared to the nucleus Coulomb one is added. This wave function variation can furthermore be used to evaluate exchange energy and exchange-energy variations due to dense plasma effects.

Finally we discuss available experimental data (albeit rare) along with different plasma potentials to estimate requested measurements precisions.

II. THE PERTURBATION METHOD

For high values of ion charges $(Z > 10)$ and relatively low quantum numbers $(n \leqslant 2)$, the ion attraction is predominant in such a way that all other interactions can be considered as perturbations for realistic experimental conditions (to be discussed further below). The general idea of the perturbation method developed below is to express the plasma effects on the electron exchange interaction as linear functionals from the plasma potentials. The kernel of the functionals can be found with the help of Coulomb Green function method and is expressed in terms of Coulomb wave functions. The final representation employs only Coulomb functions and effective plasma potentials. The constant terms in potentials can be ignored because they provide the same energy shift in the triplet and singlet terms that will cancel when calculating the difference. The approach is applicable if the Coulomb interaction is dominating over other interactions.

The advantage of this kind of representation is that one can substitute any kind of plasma potential into the functionals in order to obtain scaling laws for the dense plasma effects (in terms of plasma parameters and atomic parameters) as well as to estimate the magnitude of the effects under consideration.

Let us find the change $\delta R(r)$ in atomic functions due to a small correction $\delta U\,(r)$ to the Coulomb potential. The Schrödinger equation for the wave function is

$$(L_r - \delta U + E)(R^0 + \delta R) = 0, \tag{1}$$

where L_r is a pure Coulomb term,

$$L_r = \frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{l(l+1)}{r^2}\right] + \frac{Ze^2}{r}, \tag{2}$$

and R^0 is a pure Coulomb wave function satisfying the equation

$$(L_r + E_n)R^0(r) = 0. \tag{3}$$

δR is the correction to R^0 due to the perturbation potential δU. The energy in Eq. (1) is corrected by an amount δE,

$$E = E_n + \delta E. \tag{4}$$

We note that all these corrections are small at distances of the order of the atomic size; they are not small at larger distances. This limitation is of no real importance as only the $n = 2$ resonance and intercombination lines are of practical interest.

The Coulomb wave functions are given by

$$R^0_{nl}\,(r) \;=\; \frac{2\,Z^{3/2}}{n^2\,a_0^{3/2}}\;F_{nl}\left(\frac{2Zr}{n\,a_0}\right), \tag{5}$$

where n, l, and a_0 are the principal quantum number, the orbital quantum number, and the Bohr radius, respectively. $F_{nl}\,(x)$ are expressed in terms of normalized Laguerre polynomials [15,16]:

$$F_{nl}\,(x) = \sqrt{\frac{(n-l-1)!}{[(n+l)!]^3}}\,e^{-x/2}x^l\,L^{2l+1}_{n+l}\,(x)\,. \tag{6}$$

The Laguerre polynomials are defined as [15,16]

$$L^{2l+1}_{n+l}\,(x) = -\,[(n+l)!]^3 \times \sum_{k=0}^{n-l-1}\frac{(-x)^k}{k!\,(n-l-1-k)!\,(2l+1+k)!}. \tag{7}$$

Combining Eqs. (1), (3), and (4), we obtain the equation for the correction to the Coulomb wave function:

$$(L_r + E_n)(\delta R) = \delta U'(r)R^0(r). \tag{8}$$

The modified potential $\delta U'$ is

$$\delta U'(r) = \delta U(r) - \delta E. \tag{9}$$

Equation (8) is a nonuniform Schrödinger equation with a Coulomb Hamiltonian on the left-hand side. The solution can be found by the Green function method using the well known expression for radial Coulomb Green function $g_{nl}(r,r')$ satisfying the equation [15,16]

$$(L_r + E_n)g_{nl}(r,r') = \frac{\delta(r-r')}{rr'}. \tag{10}$$

Solution of Eq. (10) is an analytical expression for the reduced (with extraction of singularities) Coulomb Green function [16]:

$$g_{nl}(r,r') = \frac{4Z}{n\,a_0^2 e^2} \sum_{\substack{k=l+1\\(k\neq n)}}^{\infty} \frac{F_{kl}(2Zr/n\,a_0)\;F_{kl}(2Zr'/n\,a_0)}{k-n} + \frac{n^2\,a_0}{Z^2\,e^2}\left[\frac{5}{2}R^0_{nl}(r)R^0_{nl}(r') \;+\; r\,\frac{dR^0_{nl}(r)}{dr}R^0_{nl}(r') + R^0_{nl}(r)r'\frac{dR^0_{nl}(r')}{dr'}\right]. \qquad (11)$$

Solving Eq. (8) by Green function method one obtains

$$\delta R_{nl}(r) = \int_0^\infty dr'\,r'^2\,g_{nl}(r,r')\;\delta U(r')\;R^0_{nl}(r'). \qquad (12)$$

As we have pointed out in the beginning, a constant term in the potential of Eq. (12) is ignored (only energy differences are considered) and we have replaced the potential $\delta U'$ by δU. As we can see from Eq. (9), the two potentials differ by a constant amount δE.

The next step is to express the exchange energy in terms of atomic wave functions. Two expressions are to be tested: the first one is based on the statistical approach for an exchange-energy term using the free electron gas approach and the second one is deduced from direct calculations of the exchange energy for a two electron system.

A. Statistical approximation to the exchange energy

The most frequently used expression for the exchange energy is the one established for a free electron gas [15,17]. Although this approach is established for a many electron system, it is also commonly used to estimate a few electron system. The expression for the exchange energy takes the form

$$E_x = -\frac{3}{2}e^2\alpha\int_0^{R_0}\left(\frac{24}{\pi}n_b\right)^{1/3} r^2\,R^2_{nl}(r)\,dr, \qquad (13)$$

where $\alpha = 1,\ 2/3$ is a numerical constant depending on a specific choice of atomic model, n_b is the atomic electron density [15]

$$n_b\,(r) = \frac{1}{4\pi}\sum_{n,l} w_{nl}\,R^2_{nl}\,(r)\,, \qquad (14)$$

and w_{nl} is the number of electrons in the shell n.

As concerns our case of the resonance (W) and intercombination (Y) line, a configuration with one electron in $1s$ shell and another one in the $2p$ shell is of particular interest. The exchange energy deduced from Eqs. (13) and (14) is then

$$E_x = -\frac{3}{2}e^2\alpha\left(\frac{6}{\pi^2}\right)^{1/3} \times \int_0^{R_0} dr\;r^2\left[R^{2/3}_{10}(r)R^2_{21}(r) + R^{2/3}_{21}(r)R^2_{10}(r)\right]. \qquad (15)$$

When formula (15) is applied to isolated helium-like aluminum (in vacuum), we obtain a value of 167 eV for the exchange energy which is far from the value of the NIST data of 10.18 eV [18] and recent space resolved measurements in a laser produced plasma gave 9.9 ± 0.05 eV in the far target emission [4] (which are not yet understood but might also hint for dense plasma effects on the exchange energy).

We therefore conclude that the statistical model is not suitable (not even for rough estimates) to investigate dense plasma effects on the exchange energy of a two-electron system.

B. Exchange energy in two-electron system

Direct calculation of the exchange energy starts from the general expression of the exchange part of Coulomb energy matrix element for two-electron system in states ψ_1 and ψ_2 (see [15]):

$$E_x = \iint d\mathbf{r}_1\,d\mathbf{r}_2\;\psi_1^*(\mathbf{r}_1)\;\psi_2^*(\mathbf{r}_2)\;\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}\psi_2(\mathbf{r}_1)\;\psi_1(\mathbf{r}_2). \qquad (16)$$

It should be noted that we employ uncorrelated unscreened wave functions in order to obtain manageable analytical expressions rather than extreme precision data (which are physically inconsistent despite the current uncertainties for the model plasma potential expressions). The numerical evaluation Eq. (16) is usually based on the spherical symmetry of the wave functions. Expanding the interaction potential in Eq. (16) into Legendre polynomials and series of radius $r_>$ and $r_<$ (being the larger and smaller values of r_1 and r_2, respectively, see [15] for details) and using the representation of angular dependences of wave functions in Legendre polynomials one obtains after some calculations

$$E_x = \frac{2e^2}{3}\int_0^\infty dr_1\,R_{10}(r_1)\,R_{21}(r_1)\int_0^{r_1} dr_2 r_2^3\,R_{10}(r_2)\,R_{21}(r_2). \qquad (17)$$

The application of perturbation theory expresses the wave functions as

$$\begin{aligned} R_{10}(r) &= R^0_{10}(r) + \delta R_{10}(r),\\ R_{21}(r) &= R^0_{21}(r) + \delta R_{21}(r)\ , \end{aligned} \qquad (18)$$

where the upper index 0 indicates pure Coulomb wave functions. Correspondingly, the exchange energy consists of a pure Coulomb term and a perturbed term:

$$E_x = E^0_x + \delta E_x. \qquad (19)$$

The zero term in Eq. (19) is given by Eq. (17) substituting pure Coulomb functions. The second (correction) term is obtained by substituting Eq. (18), combined with Eq. (12), into Eq. (17), and then subtracting a term corresponding to E^0_x. The result is

$$\delta E_x = \frac{2}{3}e^2\left[\int_0^\infty dr_1\,f(r_1)\int_0^{r_1} dr_2 r_2^3\,R^0_{10}(r_2)R^0_{21}(r_2) + \int_0^\infty dr_1\,R^0_{10}(r_1)R^0_{21}(r_1)\int_0^{r_1} dr_2 r_2^3\,f(r_2)\right], \qquad (20)$$

where

$$f(r) = R^0_{21}(r)\int_0^\infty dr'r'^2 g_{10}(r,r')R^0_{10}(r')\delta U_{10}(r') + R^0_{10}(r)\int_0^\infty dr'r'^2 g_{21}(r,r')R^0_{21}(r')\delta U_{21}(r'), \qquad (21)$$

here δU_{10} and δU_{21} are potentials acting on $1s$ and $2p$ electrons, respectively. The indexes are introduced to distinguish between potentials acting on each electron. These potentials are different, for instance, if the interaction involves the screening between bound electrons (to be discussed in the next paragraph). These indexes can be omitted if only plasma effects are involved.

Equation (20), combined with Eq. (21), represents the change of exchange energy due to the presence of any potential (being small as compared with the Coulomb one). These equations express the relative exchange energy in terms of integrals of potential variations and Coulomb functions.

The effective values of the electron radius are just determined by the size of atomic electron orbits (wave functions). So it is natural to introduce dimensionless variables following the structure wave function given by Eq. (5). To be more specific, we limit ourselves to the $1s2p$ configuration for which the dimensionless variable $x = Zr/a_0$ is appropriate. Introducing this variable into Eqs. (20), (21), and (11) one obtains with account of Eq. (5)

$$\delta E_x = \frac{4}{3Z}\left[\int_0^\infty dx_1 f(x_1) \int_0^{x_1} dx_2 x_2^3 F_{10}(2x_2) F_{21}(x_2) + \int_0^\infty dx_1 F_{10}(2x_1) F_{21}(x_1) \int_0^{x_1} dx_2 x_2^3 f(x_2)\right], \quad (22)$$

where

$$f(r) = 2\,F_{21}(x)\int_0^\infty dx' x'^2 g_{10}(x,x') F_{10}(2x') \delta U_{10}(x') + 2\,F_{10}(2x)\int_0^\infty dx' x'^2 g_{21}(x,x') F_{21}(x') \delta U_{21}(x'), \quad (23)$$

$$g_{10}(x,x') = \sum_{k=2}^{\infty} \frac{1}{k-1} F_{k0}(2x) F_{k0}(2x') + \frac{5}{2} F_{10}(2x) F_{10}(2x') + 2x \frac{dF_{10}(2x)}{dx} F_{10}(2x') + F_{10}(2x) 2x' \frac{dF_{10}(2x')}{dx'}, \quad (24)$$

$$g_{21}(x,x') = \frac{1}{2}\sum_{k=3}^{\infty} \frac{1}{k-2} F_{k1}(x) F_{k1}(x') + \frac{5}{4} F_{21}(x) F_{21}(x') + x \frac{dF_{21}(x)}{dx} F_{21}(x') + F_{21}(x) x' \frac{dF_{21}(x')}{dx'}. \quad (25)$$

III. CORRECTION TO EXCHANGE ENERGY DUE TO ELECTRON SCREENING IN ISOLATED ION

We can validate our perturbation method by computing the correction to the exchange energy due to the electron screening effect inside the ion. Equation (22) takes into account the exchange-energy correction due to any additional potential. The zero order approximation for electron exchange energy is the one described by Eq. (17) with Coulomb functions. It predicts exchange energy for the case of a He-like Al ($Z = 13$) ion equal to 6.036 eV. The measured quantity is the difference between singlet and triplet electronic terms. This difference is equal to twice the exchange energy calculated above, that is, 12.07 eV. This value is still far from the NIST data [18]: 10.18 eV. In order to demonstrate the efficiency of the present perturbation method it is of interest to find the correction to the zero order exchange energy due to electron screening inside the isolated He-like ion.

This can be performed using the general expression for the Coulomb potential produced by bound electrons inside the ion [17]

$$\phi_b(r) = -4\pi e\left[\frac{1}{r}\int_0^r dr' r'^2 n_b(r') + \int_r^\infty dr' r' n_b(r')\right] \quad (26)$$

and substituting the bound electron density

$$n_b(r) = \sum_l (2l+1)|R_{nl}^0(r)|^2 \quad (27)$$

determined by Coulomb radial wave functions. For our case of $2p$-$1s$ transitions in He-like ions it means that one has to use the 1s-shell wave function for the screening of the $2p$ electron and the $2p$-shell wave function for the screening of 1s electron in order to avoid self-screening effects. Substituting the bound electron density Eq. (27) into Eq. (32) we obtain the screening potential and additional perturbation $\delta U(r) = -e\phi(r)$ entering into wave function corrections in Eq. (12). Making a transformation from radial functions $R_{nl}(r)$ to dimensionless functions $F_{nl}(x)$ one can see from Eqs. (22) and (23) that the screening correction from the bound electrons does not depend on Z. Using the correction $\delta U(x)$ in Eqs. (22)–(25) the correction to the difference between triplet and singlet levels in He-like aluminum ion equal to $2\,\delta E_X = -2.14$ eV. Therefore the difference itself is equal to $(12.07 - 2.14)$ eV $=$ 9.93 eV. This means that the employed perturbation method reproduces the exchange-energy shift with a precision near 1.5%. This precision is excellent remembering that other small corrections, for example, due to spin-orbit and spin-spin interactions, relativistic effect, and masses have yet to be added.

It is important to note that the present way of calculation of the electron screening is essentially motivated by the final aim to obtain analytical expressions afterward for different plasma potentials rather than to provide the highest state of the art calculation of screening effects in isolated ion atomic physics. As the results demonstrate, an overall acceptable precision is obtained with the proposed perturbation method for the screening corrections to the exchange energy.

IV. FINITE TEMPERATURE ION SPHERE MODEL

The potential variation expressed in Eq. (23) can represent any additional potential to the Coulomb one, for example, the bound electrons interaction or external potentials produced by the plasma. In this section we consider a finite temperature ion sphere model (ISM) potential. The system is represented by a sphere of radius R_0 containing the ion at the center, surrounded by bound and free electrons. The central equation of this model is the equilibrium charge distribution of the free electrons:

$$n_f(r) = n_f(R_0)\frac{4}{\sqrt{\pi}}\int_{P_0(r)}^{\infty} dp\,\frac{p^2}{(2m_e k_B T)^{3/2}} \times \exp\left\{-\frac{1}{k_B T}\left[\frac{p^2}{2m_e} - e\phi(r)\right]\right\}, \tag{28}$$

where $n_f(R_0)$ is free electron density at the distance R_0 and P_0 is a minimum momentum value taken by the free electrons. This ensures that the kinetic energy is larger than the potential energy

$$P_0(r) = \sqrt{2m_e\, e\,\phi(r)}. \tag{29}$$

The total potential is a sum of ion, free, and bound electrons potentials

$$\phi(r) = \frac{Ze}{r} + \phi_b + \phi_f. \tag{30}$$

The ion sphere radius is

$$R_0 = \left(\frac{4\pi n_i}{3}\right)^{-1/3}. \tag{31}$$

The potentials ϕ_b and ϕ_f are potentials of bound and free electrons, respectively. These potentials are linked to the bound and free electron densities n_b and n_f by the Laplace equation. For a spherically symmetric distribution of charges, the Laplace equation reduces to an integral equation for both potentials:

$$\phi_{b,f}(r) = -4\pi e\left[\frac{1}{r}\int_0^r dr' r'^2 n_{b,f}(r') + \int_r^{R_0} dr' r' n_{b,f}(r')\right]. \tag{32}$$

Assuming global neutrality of the sphere

$$Z - N_b = \int_0^{R_0} 4\pi r^2 n_f(r) dr, \tag{33}$$

N_b is the number of bound electrons that is supposed to be small as compared with the nuclear charge Z.

We suppose that the value R_0 is large as compared with the radius of the atomic electron orbit with principal quantum number n:

$$R_0 \gg a_0\frac{n^2}{Z}, \quad \text{or} \quad n_e \ll \frac{3Z^4}{4\pi a_0^3 n^6} = 1.6\times 10^{28}\text{cm}^{-3}\frac{Z^4}{n^6}. \tag{34}$$

The inequality (34) indicates that for the experimental conditions of laser produced plasma experiments [2] ($n = 2$, $Z = 13$) the free electron density should be $n_e \ll 10^{27}$ cm^{-3} which is almost always satisfied. Even for $n = 5$, the perturbation method is applicable up to solid density. It follows from Eq. (34) that dense plasma effects on the atomic functions take place at far distances from the Coulomb center where the atomic wave functions decrease exponentially.

For the general case of finite temperature ISM Eqs. (28), (32), and (33) are solved self-consistently. However, analytical solutions can be found at the limiting cases of high and low temperatures. For this purpose, the integral in Eq. (28) is simplified as follows:

$$n_f(r) = n_f(R_0)\frac{2}{\sqrt{\pi}}\int_0^{\infty} dt\,\sqrt{t + \frac{e\phi(r)}{k_B T}}\;e^{-t}. \tag{35}$$

Since the t variable is of order of unity, the integral in (35) can be calculated in closed form for both high and low temperature limit. In the high temperature limit we have

$$\frac{e\phi(r)}{k_B T} \ll 1 \tag{36}$$

and expression (35) simplifies to

$$n_f(r) = n_f(R_0). \tag{37}$$

$n_f(R_0)$ is close to the unperturbed electron density n_e [19]. We have thus

$$n_f(r) = n_e. \tag{38}$$

The particular case of an infinite temperature is called uniform electron gas model (UEGM) where the free electron density inside the atom is constant. The potential in (36) is given by Eq. (30). It consists of a potential produced by the nucleus of charge Z screened by bound and free electrons. We assume (as an approximation) that an average of N_b electrons screen this potential. The resulting potential is equivalent to the one produced by an effective charge of $Z - N_b$:

$$\phi(r) \approx \frac{(Z - N_B)e}{r}. \tag{39}$$

Condition (39) holds especially for the mean atomic radius

$$\langle r\rangle = \frac{n^2}{Z}a_0. \tag{40}$$

If we substitute (40) into (39), the condition (36) writes

$$k_B T \gg \left(\frac{Z - N_b}{n}\right)^2\frac{e^2}{a_0} \approx \left(\frac{Z}{n}\right)^2\frac{e^2}{a_0}. \tag{41}$$

The low temperature limit corresponds to the opposite inequality of relation (41)

$$k_B T \ll \left(\frac{Z}{n}\right)^2\frac{e^2}{a_0}. \tag{42}$$

Under conditions (34) and (42) one can simplify the integral in Eq. (35):

$$n_f(r) = n_e\frac{2}{\sqrt{\pi}}\sqrt{\frac{e^2(Z - N_b)}{k_B T\; r}}. \tag{43}$$

We can combine the limiting cases of large and small temperatures by using a simple fitting formula incorporating both low and high temperature limits:

$$n_f(y) \approx n_e\left(1 + \frac{2}{\sqrt{\pi y}}\right), \tag{44}$$

with

$$y = \frac{k_B T\; r}{e^2(Z - N_b)}. \tag{45}$$

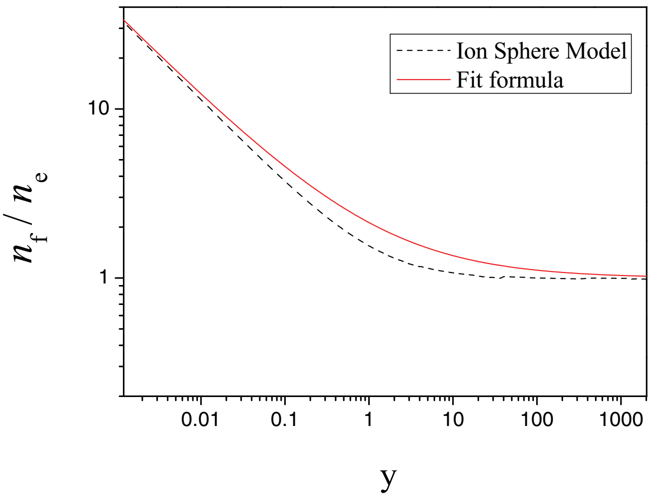

FIG. 1. (Color online) The free electron density as a function of dimensionless radius y. Comparison between ISM and fitting formula Eq. (44).

The comparison between self-consistent numerical calculations (solving simultaneously the multiconfiguration Dirac-Fock and the Poisson equation [3]) and the fitting formula (44) is presented in Fig. 1. Figure 1 shows a quite good overall agreement even for intermediate temperature values that provides the direct proof of the sufficient precision (from the atomic physics point of view) obtained by the present method.

A transformation of Eq. (32) to dimensionless variables y provides the result for the electron potential at any finite temperature, which is not known in the literature:

$$\phi(y) = -4\pi\, e\, n_e \left(\frac{Z}{T}\right)^2 \left[\frac{1}{y}\int_0^y dx' x'^2 n_f(x') + \int_y^{y_0} dx' x' n_f(x')\right] \tag{46}$$

with

$$y_0 = \frac{R_0\, k_B T}{e^2 (Z - N_b)}. \tag{47}$$

Using the analytical formula (44) we arrive at

$$\phi(y) \approx -4\pi\, e\, n_e \left[\frac{e^2(Z-N_b)}{k_B T}\right]^2 \left(\frac{y_0^2}{2} + \frac{4}{3\sqrt{\pi}} y_0^{3/2} - \frac{y^2}{6} - \frac{8}{15\sqrt{\pi}} y^{3/2}\right). \tag{48}$$

The potential (48) is of interest for all values of the variable y including the transition from high to low temperature regimes. It is convenient to employ a dimensionless atomic shell size variable

$$x = \frac{Z\, r}{a_0} = \frac{e^2 Z (Z - N_b)}{a_0\, k_B T} y. \tag{49}$$

In terms of this variable, the potential energy $\delta U_{\rm ISM} = -e\phi$ describing dense plasma effects takes the form

$$\delta U_{\rm ISM}(x) \approx 4\pi\, e^2\, n_e \left(\frac{R_0^2}{2} + \frac{4\, S\, e\, Z^{1/2}}{3\sqrt{\pi k_B T}} R_0^{3/2} - \frac{a_0^2}{6Z^2} x^2 - \frac{8\, e\, S\, a_0^{3/2}}{15 Z \sqrt{\pi k_B T}} x^{3/2}\right). \tag{50}$$

S is a screening factor which has a value of

$$S = \sqrt{1 + \frac{N_b}{Z}} = 0.92 \tag{51}$$

for helium-like aluminum ($Z = 13$ and $N_b = 2$).

In order to obtain the plasma screening one needs to substitute the plasma screening potential Eq. (50), into the general set of Eqs. (22)–(25). We recall that the constant part in Eq. (50), that is the first and the second term, do not contribute to the exchange-energy separation. It can be seen that the difference between singlet and triplet pairs in vacuum and plasma is linear in electron density

$$2\, \delta E_x[\mathrm{eV}] = -k(Z,T)\ n_e[\mathrm{cm}^{-3}] \tag{52}$$

with

$$k(Z,T) \approx 10^{-25}[\mathrm{cm}^3] 2\mathrm{Ry} \left(\frac{23}{Z^3} + \frac{11.6}{Z^2 \sqrt{T[\mathrm{eV}]/2\mathrm{Ry}}}\right). \tag{53}$$

To obtain Eq. (53) we have substituted numerical values for matrix elements of x^2 and $x^{3/2}$ arising after substitution of Eq. (49) into Eqs. (22)–(25). Equation (53) is valid for the $1s2p$ configuration in every He-like ion with nuclear charge Z for any temperature but restricted by condition (34). The first term in (53) corresponds to the infinite temperature limit and the second term to the low temperature limit.

V. DEBYE MODEL

Another standard approach to describe dense plasma effects is based on the Debye screening potential

$$V_D = -\frac{Z\, e^2}{r} e^{-r/\lambda_D} \tag{54}$$

with

$$\lambda_D = \sqrt{\frac{k_B T}{4\pi\, n_e\, e^2\, Z_{\rm eff}(T)}} \quad \text{and} \quad Z_{\rm eff}(T) = 1 + \langle Z^2\rangle / \langle Z\rangle, \tag{55}$$

where the effective ion charge $Z_{\rm eff}$ was introduced in terms of the averaged charge and its squared average. It turns out that one does not need the total Debye potential but only the difference between the Coulomb and the Debye potentials. This difference is a small correction to the Coulomb potential. It is also natural to express the correction in terms of the dimensionless parameter x:

$$\delta U_D(x) = -\frac{Z\, e^2}{r}(e^{-r/\lambda_D} - 1) \approx \frac{Z\, e^2}{\lambda_D} - \frac{a_0\, e^2}{2\, \lambda_D^2}\, x. \tag{56}$$

All plasma potentials presented above are considered to be small as compared with the Coulomb potential inside the ionic shell under consideration. The condition allows applying the perturbation theory developed below.

In order to work out explicit results for the Debye screening model we substitute the Debye screened potential (56) into the general formulas (22)–(25). The result takes the form

$$2\,\delta E_x[\text{eV}] = -k(T)\ n_e[\text{cm}^{-3}], \tag{57}$$

$$k(T) = 10^{-25}[\text{cm}^3]\ 2\text{Ry}\frac{11.5\ Z_{\text{eff}}(T)}{Z\ \ T[\text{eV}]/2\text{Ry}}. \tag{58}$$

The numerical factor in Eq. (58) is much larger as compared with Eq. (53) for the ISM due to less strong dependence on nuclear charge Z [compare with Eq. (53)].

VI. DISCUSSION OF AVAILABLE THEORETICAL AND EXPERIMENTAL DATA

Figure 2 displays the coefficient k of Eq. (53) for He-like aluminum ions ($Z = 13$) in comparison with data published in [3]. A good correspondence between the results from the present perturbation theory and the self-consistent numerical solutions of the multiconfiguration Dirac-Fock and Poisson equation is obtained: the two results agree extremely well at the high temperature and low temperature limit and make a difference of only about 10% at intermediate values of y (temperatures ~50 eV). This small difference is due to the analytical representation of Eq. (44). We note that Eq. (44) can be made more precise but this will only result in small corrections to the curves presented in Fig. 2. We can therefore conclude that the present analytical presentation of the perturbation method reproduces sufficiently well the very complex numerical calculations of [3]. It should be emphasized that the explicit form of the present perturbation method employing unscreened uncorrelated wave functions has been chosen in order to obtain analytical results, scaling laws, and closed expression for any perturbation potential with a reasonable physical precision rather than obtaining state of the art atomic physics precision for imprecise plasma potentials.

The comparison of available experimental data [4] with the theoretical result for the Debye model according to Eq. (57) is presented in Fig. 3. The target distances correspond to particular sets of density and temperature [4] that have been employed to introduce the curves for the Debye model in Fig. 3. The dependence of effective ion charge on the electron temperature was calculated from non-LTE atomic population kinetics [20]. The data from the Debye screening model are located inside the large experimental error bars but do not represent any observed change with the target distance. A more detailed comparison is presented in Fig. 4 where both theoretical models are shown together with experimental data on a logarithmic scale. Neither the Debye nor the ISM represents any reasonable agreement with the data. Figures 3 and 4 indicate that the experimental precision has to be improved by at least a factor of 3 in order to derive definite conclusions about the models for the plasma potential.

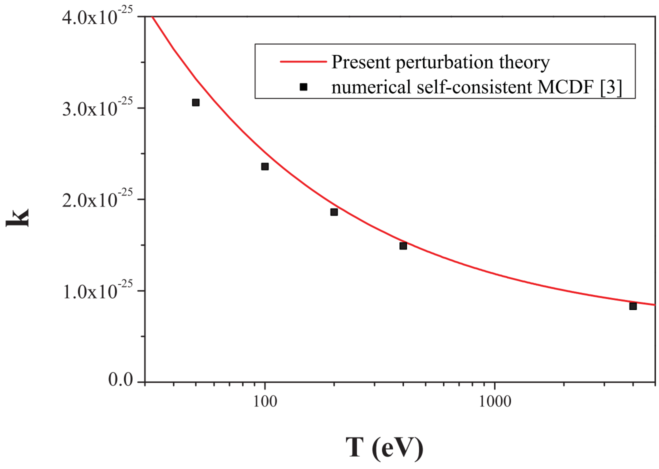

FIG. 2. (Color online) The factor $k(Z,T)$ [ISM, see Eq. (53)] vs electron temperature for He-like aluminum ion ($Z = 13$) in comparison with numerical solution of Schrödinger equation [3].

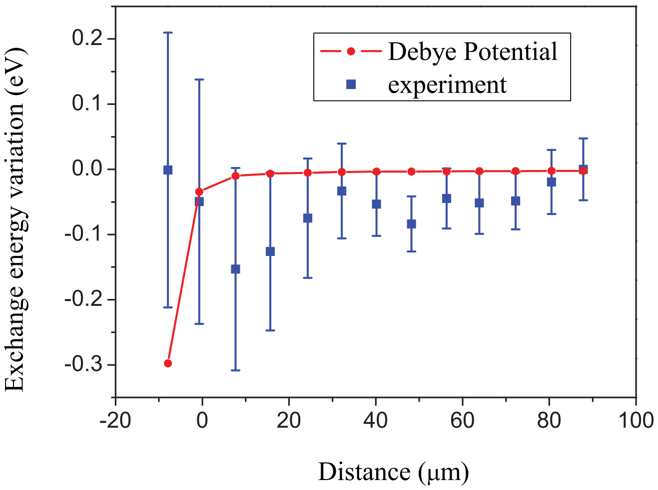

FIG. 3. (Color online) Comparison of the Debye screening model with the experimental data from [4].

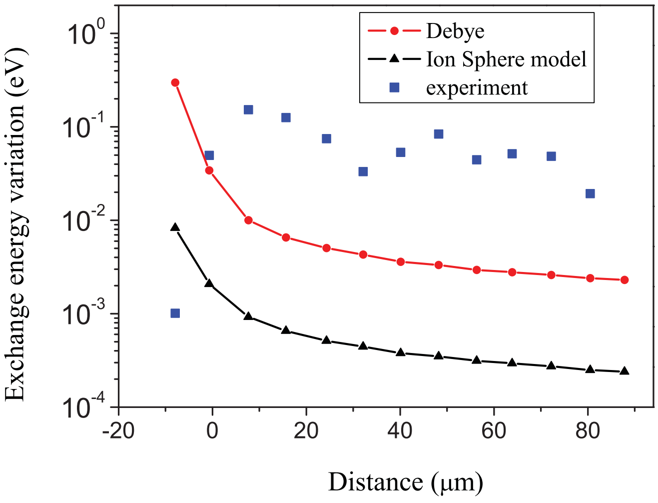

FIG. 4. (Color online) Detailed comparison between theoretical and experimental [4] data for the relative exchange-energy shift (the absolute values of energies is reported on a logarithmic scale).

VII. CONCLUSION

An alternative analytical method to calculate dense plasma effects on exchange-energy shifts ΔE_x of highly charged ions is proposed. The method is based on a perturbation theory expansion for a potential produced inside the atom by charged plasma particles. The conditions to validate the perturbation theory are easily met in usual experiments: for example, for He-like aluminum ions and $n = 2$ singlet and triplet states the limitation results in the condition $n_e \ll 10^{27}$ cm^{-3}.

Closed expressions for any arbitrary plasma potential are derived with the help of analytical expressions for Coulomb Green functions. The model expresses the relative exchange-energy shift in terms of simple functionals from hydrogen atomic wave functions and the perturbation potential. The great advantage of the present model is that it results in closed expressions for any arbitrary plasma potential to describe the plasma-atom interaction and a reasonable precision requested for dense plasma spectroscopy. This allows extracting analytical dependences on main plasma and atomic parameters (electron density n_e and temperature T as well as ion charge Z).

Detailed calculations were performed for the singlet $1s2p\,^1P_1$ and triplet $1s2p\,^3P_1$ configurations of He-like ions with a charge Z and applied to the ion sphere and Debye model. For the Debye model the analytical scaling law $\Delta E_x = A_D\, n_e\, Z_{\mathrm{eff}}/(Z\,T)$ has been obtained where Z_{eff} is the effective plasma charge and A_D is a constant.

The great power of the present method is demonstrated for the ion sphere model (ISM). Even for the finite temperature case, an analytical expression could be derived (A_I is a constant): $\Delta E_X \approx A_I n_e \{23/Z^3 + 11.6/(Z^2\sqrt{T[\mathrm{eV}]/2\mathrm{Ry}})\}$. The comparison of the present perturbation method applied to the ISM with numerical solution of the multiconfiguration Dirac-Fock equation discovered a very good correspondence.

The comparison of the present method with available data [4] indicates that the experimental precision needs to be increased by at least a factor of 3 in order to decide between different plasma potentials.

Moreover, a further general conclusion is that the present perturbation theory based on Coulomb Green functions can be considered as an extension of the well-known Z^{-1}-expansion method in atomic physics on plasma-atom interaction potentials to study dense plasma effects on the atomic structure.

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