Redshift of the Lyman-α emission line of H-like ions in a plasma environment

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We present a critical assessment of the applicability of the Debye-Hückel (DH) approximation to the redshift of the Lyman-α emission line of the H-like ions under a dense plasma environment. By carefully considering the $2p \rightarrow 1s$ transition spatially and temporally, our investigation suggests that the DH approximation may be applied to a limited number of H-like ions, such as the ones with Z between 5 and 18 or with Z greater than 50. Our numerical calculation, in fact, leads to quantitative agreement with the observed redshift of the well-isolated Lyman-α line at plasma density of the order of 1×10^{22} cm^{-3} or higher with an electron temperature of several hundred eV of H-like Al^{12+}. Our study also yields simulated data consistent with those from more elaborate quantum mechanical approaches.

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I. INTRODUCTION

At a density of 1×10^{22} cm^{-3} or higher, the laser-produced plasma is substantially higher in density than the typical gas-discharged plasma at $1 \times (10^{15} - 10^{18})$ cm^{-3}. It is not surprising that the atomic structure of the ions is influenced by such a high-density plasma environment. Indeed, it has been observed experimentally in a number of such laser-produced dense plasmas that the atomic spectral lines are redshifted at an electronic temperature of a few hundred eV or less, and at a density of 1×10^{22} cm^{-3} or higher [1–4]. Spectroscopically, the redshift of the well-isolated Lyman-α emission line of the H-like ion has always been considered as one of the better candidates for the high-density diagnostic of laser-produced plasma [5]. Qualitatively, this may be attributed, following the simple Debye-Hückel (DH) approximation [6,7], to the upward shift of the atomic energy levels due to the screened Coulomb potential in the presence of the external plasma environment. However, it was shown by Nantel *et al.* [3] that near the series limit, the DH approximation breaks down. This, of course, is expected since, first, the DH approximation is more suitable for the gas-discharged plasmas and, second, the atomic electron responsible for the atomic spectral lines near the ionization threshold is located at a distance far away from the nucleus, i.e., at a distance substantially greater than the radius of the Debye sphere. On the other hand, Fig. 1 of [3] also shows that for the spectral lines of H-like C^{5+} corresponding to transitions involving electrons in the low-n states, the DH model appears to work qualitatively just like other more elaborated models.

For the DH model and the classical Maxwell-Boltzmann statistics to apply for the specific atomic process in a dense plasma environment, one should consider carefully if the basic criteria for the DH model are satisfied in terms of the interaction region and also the characteristic time of the atomic transition. We shall consider first the key aspect in terms of the interaction region. In a recent study on the photoionization of one- and two-electron atoms subject to a plasma environment, Chang and Fang [7] have pointed out that the DH approximation could be applied to an atomic transition if the process is short ranged in nature. This applies, in general, for transitions involving the ground state of the atom since the transition rates are dictated mostly by the overlap in the transition matrix between the ground-state wave function χ_i and the final-state wave function χ_f up to a distance r_c from the nucleus (i.e., the critical interaction region), where the amplitude of the wave function of the ground state is non-negligible. This results from the fact that with a near-zero χ_i at $r > r_c$, the overlap between χ_i and χ_f beyond r_c is much smaller than that from the inner interaction region with $r < r_c$.

Temporally, the scale characteristic of the motion of the atomic electron has to be considerably different (either greater or smaller) from the correlation time τ_p, or the inverse of the plasma frequency f_p of the outside plasma [8], i.e., $\tau_p = 1/f_p$. The plasma frequency (in units of Hz) for a given plasma density n (in units of cm^{-3}) could be estimated by the simple expression $f_p = 8.977 \times 10^3 n^{1/2}$ Hz (see, e.g., Eq. (4-26) of [9]). The laser-produced dense plasma at a density of 1×10^{22} cm^{-3} is far from being a thermodynamically equilibrium system with its plasma frequency greater than 9×10^{14} Hz or with $\tau_p \sim 10^{-15}$ sec or less. This is comparable to the time for an electron revolving around the nucleus for a hydrogen atom in its ground orbit at about 1.5×10^{-16} sec and it is nearly the same for the $2p$ orbit at 1.2×10^{-15} sec. Since the rate of an atomic electron revolving around the nucleus scales like Z^2 for H-like ions, the time-scale characteristic of an atomic electron revolving around the nucleus would be at least one order of magnitude smaller than τ_p of the plasma for H-like ions with larger Z (e.g., $Z > 5$), such as the H-like Al^{12+} ion.

The other important time characteristic of the Lyman-α emission line is the time that the transition takes place or the average lifetime T_{2p} of the upper $2p$ state of the transition, which is the inverse of its transition probability A_{2p}. For H-like ions, A_{2p} could be expressed in terms of the dipole transition matrix element $d_{1s,2p} = \langle 1s \mid r \mid 2p \rangle$ and the energy

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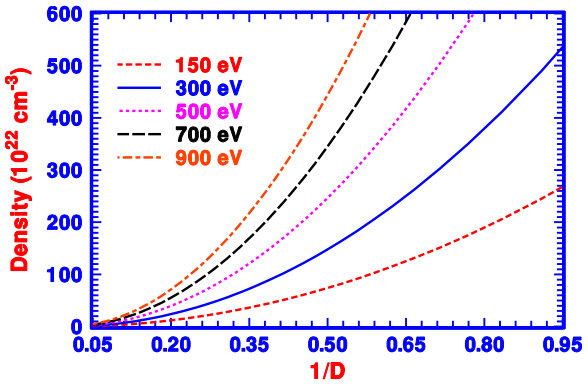

FIG. 1. (Color online) The variation of plasma density n as a function of $1/D$ at various electron energies.

separation $\delta_{1s,2p}$ between the $1s$ and $2p$ levels, or the product of $d^2_{1s,2p}$ and $\delta^3_{1s,2p}$ (see, e.g., Eq. (59.11) of [10] and more details for complex atoms in [11]). It could also be expressed as the product of the oscillator strength $f_{1s,2p}$ and $\delta^2_{1s,2p}$ (see, e.g., Eq. (59.15) of [10]). In addition, it is well known that the oscillator strength $f_{1s,2p}$ of the H-like ion remains the same as the one for the hydrogen atom. This is due to the fact that the Z-dependent parts from the $d^2_{1s,2p}$ and the $\delta_{1s,2p}$ cancel out against each other. With a constant oscillator strength $f_{1s,2p}$, the lifetime $T_{2P} = 1/A_{2p}$ of the H-like ions will thus decrease inversely proportional to $\delta^2_{1s,2p}$ or Z^4. For the Lyman emission lines of a hydrogen atom, the estimated lifetime is of the order of a nanosecond (or, more precisely, 1.6 ns for the Lyman-α line; see, e.g., Table 15 of [10]) and is substantially different from τ_p for laser-produced plasma. This leads to a lifetime for the $2p$ state about one order of magnitude or more longer than τ_p for an H-like ion with an intermediate Z (e.g., $Z < 18$). As Z increases further until it is greater than, e.g., 50, the lifetime of the np state would then be around one order of magnitude shorter or less than τ_p.

By taking into account both time characteristics of the atomic transition, together with the earlier discussion on the interaction region, one could now conclude that the DH model would only work for the Lyman-α lines for H-like ions with Z approximately between 5 and 18 or greater than 50 at density around 1×10^{22} cm^{-3}. Interestingly, we find that the existing experimental works on atomic spectra from laser-produced high-density plasma happen to be those within this range of Z, i.e., H-like Al^{12+} [1], C^{5+} [2,3], and Ar^{17+} [4]. In addition, the Lyman lines for H-like Ne^{9+} were also investigated in great detail by more elaborate simulation schemes, which take into account the ion polarization effect [8,12,13]. In particular, Nguyen *et al.* [8], based on a quantum mechanical impact theory (QMIT), have estimated the Lyman-α redshift (or polarization line shift) of H-like Ne^{9+} to be 20% greater than an earlier quantum mechanical treatment by Davis and Blaha [12] (which takes into account only partially the effect of the ion charge density). This difference, as pointed out by Nguyen *et al.*, comes essentially from the negative contribution by ions.

Following the DH approximation, the potential for an atomic electron due to a charge-neutral electron-ion plasma at a distance r from a nuclear charge Z is given by [13,14]

$$V_d(r;D) = \begin{cases} V_i(r) = -Ze^2\left(\frac{1}{r} - \frac{1}{D+A}\right), & r \leqslant A \\ V_o(r) = -Ze^2\left(\frac{De^{A/D}}{D+A}\right)\frac{e^{-r/D}}{r}, & r \geqslant A, \end{cases} \tag{1}$$

where A is the radius of the Debye sphere and D is the Debye length. Any estimate of the plasma effect on the atomic process based on the DH approximation should be limited to Debye lengths that are greater than A. Nearly all recent applications [15–21] of the DH approximation to atomic processes were carried out in the limit when $A \to 0$, i.e., with a screened Coulomb potential V_s in a one-electron Hamiltonian $h_o(r,D)$,

$$h_o(r;D) = \frac{p^2}{2m} + V_s(r;D) \quad \text{and} \quad V_s(r;D) = -\frac{Ze^2}{r}e^{-r/D}, \tag{2}$$

where p is the momentum of the electron.

In the present study, the atomic orbital functions of the H-like ion for the initial and final states of the transition, i.e., χ_i and χ_f, are generated, instead, by

$$\left[\frac{p^2}{2m} + V_d(r;D)\right]\chi_{n\ell}(r;D) = \epsilon_{n\ell}(D)\chi_{n\ell}(r;D). \tag{3}$$

The energy of the Lyman-α line is then given by

$$\delta_{L_\alpha}(D) = \epsilon_{2p}(D) - \epsilon_{1s}(D) \tag{4}$$

and, accordingly, the redshift of the Lyman-α line can be expressed as

$$\Delta_\alpha(D) = \delta_{L_\alpha}(D=\infty) - \delta_{L_\alpha}(D), \tag{5}$$

where $\delta_{L_\alpha}(D=\infty)$ is the plasma-free energy of the Lyman-α line.

Under the DH approximation, the screening of the nuclear charge experienced by the atomic electron due to the outside plasma is characterized by the Debye length. It is given in units of Bohr radius a_o, in terms of the plasma temperature T (in degree Kelvin) and density n (in cm^{-3}), respectively, by (see also, e.g., Eq. (2.5) of [14])

$$D = 1.304 \times 10^9 (T/n)^{1/2} a_o. \tag{6}$$

[Please note that in Eq. (2) of [7], 10^8 should read 10^9.] Alternatively, it can be expressed by $D = 6.90(T/n)^{1/2}$ in units of cm. For the laser-produced dense plasmas (e.g., H-like C^{5+}, Al^{12+}, and Ar^{17+}), it may be more convenient to express the Debye length D in terms of the electron energy k_bT in units of eV and its density in units of 1×10^{22} cm^{-3} by the expression of (see also, e.g., Eq. (1-17) of [9])

$$D = 1.4048(k_bT/n)^{1/2} a_o. \tag{7}$$

Figure 1 presents the variation of plasma density n as functions of $1/D$ at various electron energy k_bT, where k_b is the Boltzmann constant. We should point out that in some applications of the DH approximation [15,16], an extra factor $4\pi(Z+1)$ is added to the density n by assuming the same mobility for ions and electrons, which does not apply to the subject of interest in this study.

Our preliminary calculations to examine qualitatively and quantitatively the redshifts of the Lyman lines for hydrogen-like systems have suggested that the numerically simulated

redshifts are actually fairly sensitive to the choice of A. One of the main purposes of this work is to present a more detailed analysis of the redshift of the Lyman-α line for H-like systems subject to a plasma environment based on a number of schemes with different choices of the radius of Debye sphere A, which we will outline in Sec. II. We will present our quantitative results and compare the simulated redshifts with the available observed data in Sec. III. We will show that by varying the two key parameters (i.e., D and A) under DH approximations, we are able to obtain the redshift of the Lyman-α line of H-like Al^{12+} that is consistent with the only experimentally observed value [1]. Our results are also consistent with simulated redshifts for the Lyman-α line of H-like Ne^{9+} derived from the earlier in-depth studies [8,12]. A conclusion of our study will be presented in Sec. VI.

II. NUMERICAL SIMULATION WITH DEBYE-HÜCKEL APPROXIMATION

As we pointed out earlier, the Debye-Hückel approximation, with its simplicity, is able to qualitatively attribute the redshifts of the Lyman lines to the upward shift of the atomic energy levels due to the presence of the potential subject to the plasma environment given by Eq. (1). The question we would like to address is whether it could also lead to quantitative estimation that is consistent with the observed data for H-like ions within the range of Z where the DH approximation is applicable as we pointed out earlier.

We started our investigation, like many recent applications of DH approximation to atomic processes, by first setting $A = 0$ as the limiting case to simulate the redshifts. In addition to this first choice, one could also expect that the value A changes as D varies, i.e., A may depend upon the plasma density and temperature. A judicious determination of the relation between A and D would require a far more elaborate analysis and the DH approximation would no longer be the simple model as it is. To keep our investigation simple, our second *ad hoc* choice is to set A to be γ times smaller than the value of D. That is, by choosing $A = D/\gamma$ (e.g., with $\gamma = 10$, A is one order of magnitude smaller than D), we may be able to find out how the resulting redshifts vary as D changes and if this somewhat arbitrary choice might offer an acceptable physical interpretation of the redshift of the Lyman emission lines of H-like ions due to a plasma environment.

As we already pointed out, the atomic transitions leading to all Lyman lines of H-like systems are essentially dictated by the $1s$ orbit. This implies that the interaction is short range in nature and is consistent with what we discussed earlier for DH approximation to apply. For the outside plasma to at least influence the $1s$ orbit, however small, one should not assume too large a value of A to have little or no plasma influence on the $1s$ orbit. At the same time, the value of A should not be too small so that the entire $1s$ orbit is exposed to the outside plasma field to the extend that it loses the atomic characteristics entirely. As a result, our third choice in simulating the redshifts of the Lyman lines is to set A to be at least the average size of the H-like ions in its $1s$ orbit [i.e., $A_{\min} = (1/Z)a_o$] but no greater than twice the size of the ions [i.e., $A_{\max} = (2/Z)a_o$]. In other words, our last choice is to set $A = (\eta/Z)a_o$ for the H-like systems with a nuclear charge Z, where $\eta_{\min} = 1$ and $\eta_{\max} = 2$.

TABLE I. The redshifts of the Lyman-α line for hydrogen Δ_α as functions of *reduced Debye length* λ_D for $\gamma = 20$ and $\eta = 0, 2.0, 1.5$, and 1.0, respectively.

	$\Delta_\alpha\ [a(n) = a \times 10^n$ eV]				
$\lambda_D\ (a_o)$	$\gamma = 20$	$\eta = 0.0$	$\eta = 2.0$	$\eta = 1.5$	$\eta = 1.0$
1000	0	5.000(−5)	3.000(−5)	3.000(−5)	4.000(−5)
400	0	3.000(−4)	1.600(−4)	2.000(−4)	2.500(−4)
300	0	5.300(−4)	2.900(−4)	2.600(−4)	4.400(−4)
200	0	1.180(−3)	6.400(−4)	8.100(−4)	9.800(−4)
100	4.200(−4)	4.650(−3)	2.520(−3)	3.180(−3)	3.850(−3)
80	1.250(−3)	7.220(−3)	3.910(−3)	4.920(−3)	5.970(−3)
60	3.990(−3)	1.271(−2)	6.850(−3)	8.650(−3)	1.050(−2)
50	7.510(−3)	1.816(−2)	9.760(−3)	1.233(−2)	1.499(−2)
40	1.500(−2)	2.806(−2)	1.500(−2)	1.899(−2)	2.313(−2)
35	2.191(−2)	3.638(−2)	1.938(−2)	2.456(−2)	2.995(−2)
30	3.301(−2)	4.902(−2)	2.601(−2)	3.301(−2)	4.030(−2)

All three choices proposed above have the advantage to transform the potential given by Eq. (1) to scale as Z^2 if we define the Debye length D in terms of a *reduced Debye length*,

$$\lambda_D = ZD. \tag{8}$$

For example, with $A = (\eta/Z)a_o$, V_d from Eq. (1) will be proportional to Z^2 in the form of

$$V_d(\rho;\lambda_D) = \begin{cases} V_i(\rho) = -(Ze)^2\left(\frac{1}{\rho} - \frac{1}{\lambda_D+\eta}\right), & r \leqslant A \\ V_o(\rho) = -(Ze)^2\left[\frac{\lambda_D e^{\frac{\eta}{\lambda_D}}}{(\lambda_D+\eta)}\right]\frac{e^{-\frac{\rho}{\lambda_D}}}{\rho}, & r \geqslant A. \end{cases} \tag{9}$$

Since the radial parts of the orbital wave functions, χ_i and χ_f, for H-like systems also depend on $\rho = Zr$, we could expect that the resulting energy values and the redshifts scale as Z^2.

III. RESULTS AND DISCUSSIONS

Following the discussion earlier, the redshifts derived from the current study depend on two parameters, i.e., first, a temperature- and density-dependent Debye length D and, second, a dimensionless parameter, γ or η, which is linked to the radius of the Debye sphere A, in terms of either $A = D/\gamma$ or $A = (\eta/Z)a_o$. Table I lists the simulated redshift, Δ_α, of the Lyman-α line for hydrogen at a few selected Debye lengths with $Z = 1$, or at the reduced Debye length λ_D for $\gamma = 20$ and $\eta = 0, 1.0, 1.5$, and 2.0, respectively. As expected, with $\eta = 0$, the calculated redshift is at its maximum value as the shifts of individual energy levels are at their maxima due to the maximum Coulomb screening with $A = 0$, or when the effect of the outside plasma environment is at its strongest. As we pointed out earlier, it is interesting to note that the calculated redshift is fairly sensitive to the choice of A. For example, the redshifts with $A = 0$ (or at $\eta = 0$) have values close to twice that of the values with $A = 2a_o$ (or at $\eta = 2.0$).

Figure 2 presents our simulated Lyman-α redshifts of H-like Al^{12+} embedded in a plasma environment as functions of $1/D$ with the radius of Debye sphere A given by $\gamma = 20$, and $\eta = 0, 1.0, 1.5$, and 2.0, respectively. Our data is derived from

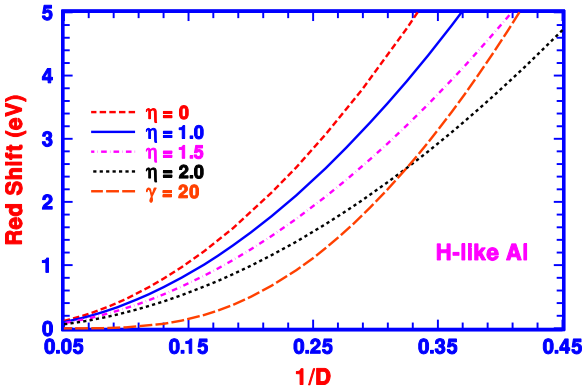

FIG. 2. (Color online) Simulated Lyman-α redshifts of H-like Al^{12+} as functions of $1/D$ with the radius of Debye sphere A given by $\gamma = 20$, and $\eta = 0, 1.0, 1.5$, and 2.0, respectively.

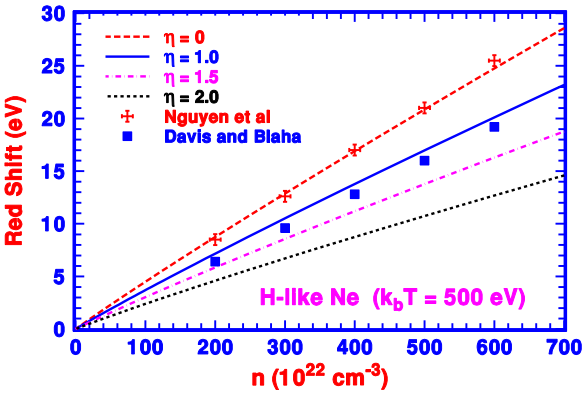

FIG. 4. (Color online) Comparison between our simulated redshifts as a function of density n at 500 eV of H-like Ne^{9+} with results from existing quantum mechanical approaches by Nguyen *et al.* [8] and Davis and Blaha [12].

more complete simulated values such as those listed in Table I for hydrogen with the Debye length D scaled as λ_D/Z and the redshifts Δ_α scaled as Z^2. Again, we find that the simulated redshifts vary substantially with different radius of Debye sphere A. To compare directly with the only quantitatively observed redshift in H-like Al^{12+} from the laser-generated plasma at an electron energy $k_bT = 300$ eV, we convert the data from Fig. 2 with Eq. (7) or those from Fig. 1 as functions of plasma density n in Fig. 3. Our simulated redshift is in good agreement with the measured value at 3.7 ± 0.7 eV and a density of $(5-10) \times 10^{23}$ cm^{-3} [1]. At $\eta = 2$, our results are also in close agreement with the simulated QMIT redshifts [1,8] at 3.5 eV and a density 8×10^{23} cm^{-3}.

We now turn our attention to the redshift of H-like Ne^{9+}. The results of the current investigation are compared in Fig. 4 with the earlier simulated data from two quantum mechanical approaches, i.e., the QMIT by Nguyen *et al.* [8] and the one by Davis and Blaha [12]. In particular, the QMIT suggested a linear dependence of the redshifts as functions of density at fixed electron energy (see Eq. (31) of [8]). Our simulated results with *ad hoc* free parameter η and that of Davis and Blaha show a density dependence that is close to linear, but they both deviate from linear slightly at higher density. As pointed out also by Nguyen *et al.*, the difference between the simulated redshifts for the H-like Ne^{9+} based on these two quantum mechanical approaches is essentially due to the insufficient negative contribution from ions. In addition, Nguyen *et al.* concluded that their calculated redshifts including the total ion polarization should be considered as the limiting ones, as shown in Fig. 4. For a charge-neutral plasma, the DH model assumes the same electron and ion density outside the Debye sphere, whereas the atomic electron is subject only to a Coulomb screened potential due to the nuclear charge Z with no positive ion charge inside the Debye sphere. With a finite radius A, i.e., with a nonzero η, effectively, only a part of the ion polarization effect due to the plasma environment is included. In other words, the full ion polarization effect is accounted for only in the limit with $A = 0$ when the atomic electron is subject to a complete Coulomb screening or a less attractive potential, resulting in a larger redshift due to the more pronounced upper lifting of the atomic energy levels. Indeed, as one would expect, our simulated results with $A = 0$ (or $\eta = 0$) agree well with the limiting values from the QMIT calculation by Nguyen *et al.* shown in Fig. 4.

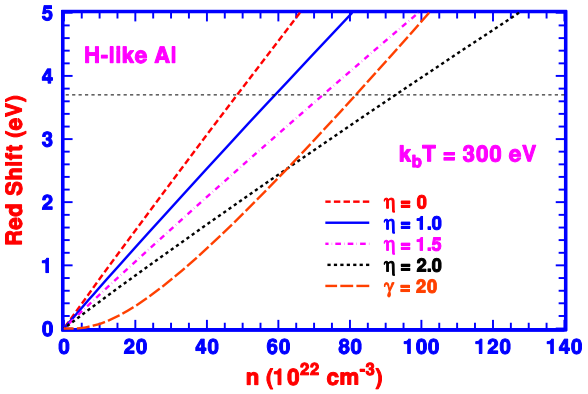

FIG. 3. (Color online) Simulated Lyman-α redshifts of H-like Al^{12+} as functions of density n at 300 eV with the radius of Debye sphere A given by $\gamma = 20$, and $\eta = 0, 1.0, 1.5$, and 2.0, respectively.

The choice we made earlier to have the value of η between $\eta_{\min} = 1$ and $\eta_{\max} = 2$, based on the spatial consideration of the interaction region, appears to also represent well the degree of ion polarization effect included in the simulated redshifts based on the DH model. With a value of η between 1.0 and 2.0, our simulated redshifts appears to agree well with the observed experimental value for H-like Al^{12+} ion shown in Fig. 3. They are also consistent with the earlier simulated results from the quantum mechanical approach by Davis and Blaha for H-like Ne^{9+} shown in Fig. 4. The simulated result with the *ad hoc* free parameter $\gamma = 20$ is not included in Fig. 4 as it fails to reproduce qualitatively the linear dependence suggested by the two earlier quantum mechanical approaches.

One of the key advantages in applying the nonrelativistic DH model to the Lyman emission lines of the H-like ions with Z approximately between 5 and 18 is the Z scaling as we discussed earlier. Obviously, the simple Z scaling will not apply if the contribution from the relativistic effects turns out to be significant. For small- to intermediate-Z ions, such as Ar^{17+}, the estimated contribution from the relativistic effects

is, in fact, minimal and generally around 1% or less (see, e.g., Tables 3 and 4 of [15]).

IV. CONCLUSION

The energy shift of an isolated atomic emission line, such as the Lyman-α line of the H-like ion, has always been considered as one of the possible candidates for the high-density diagnostic of laser-produced plasma [5]. We have shown in Sec. III that the Debye-Hückel approximation, with a judicial choice of the radius of Debye sphere, could generate the redshift of H-like ion in a plasma environment that is in agreement with the experimentally observed value, in addition to reproducing the simulated data consistent with more elaborate simulations based on quantum mechanical approaches. With the Z^2 scaling, the Debye length D derived from λ_D according to Eq. (8), and the data similar to those tabulated in Table I, it becomes extraordinarily easy to apply the DH model based on what we present in this paper to generate the data shown in Figs. 3 and 4. What is needed would be additional experimental data such as that from Ref. [1] for other ions with Z between 5 and 18 and at other electron temperatures and densities. These experimental data could then serve as the benchmark to determine the parameters of our proposed simple DH model.

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