Theory of the polarization shift of quantum levels

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The problem of calculating the energy shift of hydrogen-like levels of ions due to the polarization of free charges in a plasma is analyzed. A linearized statistical model is used to provide a self-consistent description of the screening of a nucleus by plasma charges and a localized electron. An expression asymptotic in the parameter $r_n/r_D \ll 1$ is obtained for the energy of the polarization shift (r_n is the characteristic size of the orbit of a quantum electron and r_D is the Debye radius of the plasma). These results agree well (in the range of validity of the model) both with the available experimental data for the He II ions and with the author's own numerical calculation based on a nonlinear statistical model of the screening.

1. INTRODUCTION

The problem of determining the energy of the polarization shift of quantum levels of ions and atoms in a plasma has been studied for some time (for reviews see, for example, Refs. 1–3). There is a fairly large number of approximate models which sometimes give the opposite signs for the energy of the polarization shift (Ref. 3). This is due to the difficulties encountered in a self-consistent description of the screening of the nuclear charge by a quantum electron in the presence of free electrons and ions in a plasma. The most rigorous description of the polarization shift is, in the present author's opinion, that given in Ref. 4 and based on simultaneous self-consistent solution of the nonlinear Poisson equation for the total potential and of the Schrödinger equation for a bound electron. The nonlinear relationships between the concentrations of free electrons and ions in a plasma, on the one hand, and the total potential φ, on the other, were determined in Ref. 4 by assuming classical statistics. The numerical calculations given in Ref. 4 demonstrated in particular that at very high densities (at $n_e \sim 10^{24}$ cm^{-3} in the case of the Ne VIII ions and Ly_α lines) there may be a change in the direction of the polarization shift. Only in the range of such high concentrations and at high temperatures can we use, for example, the model of screening by a "frozen-in" electron gas,[5] which predicts line shifts in the direction of shorter wavelengths. It should also be mentioned that the use of the linearization (by analogy with the Debye–Hückel screening theory) in the case of the system of equations obtained in Ref. 4 makes it possible to write down the general solution of the equation for the self-consistent potential in terms of the appropriate Green's function (see Ref. 6).

The existence of a "red" shift in the case of the $n = 4, 5, 6 \rightarrow n' = 3$ transitions in hydrogen-like He II ions was demonstrated quite clearly in the experiments reported in Ref. 7, which involved a Z-pinched discharge at moderately high plasma densities $n_e^{(0)} \sim (1\text{–}8) \times 10^{16}$ cm^{-3} at temperatures $T \sim 4$ eV. The authors proposed also a simple theoretical model for the interpretation of the experimental results based on the Debye (linear) screening model and on the assumption that the quantum electron is point-like (see below). This assumption is justified by the fact that the orbit size r_n is usually much less than the Debye plasma radius r_D. It is shown that the main term $(Z-1)/r_D$ of the series expansion of the energy of the level polarization shift is independent of the quantum numbers n and l (see also Ref. 6), so that the line shifts are governed by terms of higher order, r_n/r_D^2. Hence, it is clear that the shift of the levels should be calculated sufficiently accurately and this is indeed the reason for the failure of a number of attempts to describe the polarization shift of lines using fairly rough non-self-consistent models.

We shall use the Debye (linearized) model of the screening which allows self-consistently for the existence of a quantum electron and we shall consider the problem of calculation of the energy of the polarization shift of hydrogen-like levels in a plasma. Using the solution for the self-consistent total potential obtained asymptotically in the parameter $r_n/r_D \ll 1$, we shall obtain analytic expressions for the polarization shift of levels and we shall include terms dependent on the quantum numbers n and l. The solutions obtained, which allow correctly for the presence of a spatial distribution of the quantum electron, are valid for any nuclear charge Z of the ions, in contrast to the solution given in Ref. 7, which is valid only if $Z \gg 1$. For example, this solution makes it possible to find the polarization shift of lines of the hydrogen atom in the $Z = 1$ case, which is toward shorter wavelengths, i.e., opposite to that observed in the case of ions. It should be pointed out that in estimating the total shift of hydrogen lines we must allow for the competing mechanism of the Stark quadrupole shift of the levels (see Refs. 8 and 9).

We shall also report numerical calculations of the polarization shift in the case of a nonlinear model of self-consistent screening. In the range of validity of the Debye model, i.e., when $n \gtrsim (Z/T\,[\text{eV}])^{1/2}$ (see below), the results of numerical calculations are described well by analytic formulas derived below and are also in agreement with the experimental data reported in Ref. 7 for the $n = 4, 5, 6 \rightarrow n' = 3$ transitions in the He II ions at $T = 4$ eV when $n_e^{(0)} \sim (1\text{–}8) \times 10^{16}$ cm^{-3}.

2. FORMULATION OF THE PROBLEM

We shall analyze the polarization shift of the levels of hydrogen-like ions on the assumption that the states localized in a plasma are those with the orbit size $r_n \lesssim r_s$ [$r_s = (3/4\pi)^{1/3} (n_i^{(0)})^{-1/3}$ is the average distance between the ions in a plasma and $n_i^{(0)}$ is the equilibrium ion density]. This relationship imposes limits on the principal quantum numbers of the levels in question:

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$$n \leqslant \{8{,}8\cdot 10^3 (n_i^{(0)}\,[\mathrm{cm}^{-3}])^{-1/6}\} Z^{1/2}. \qquad (1)$$

Rydberg atoms may exchange charge with plasma ions; the process has a large characteristic cross section $\sigma_{ex} \propto \pi n^4/Z^2$. Therefore, these atoms can exist in a plasma if the relevant collision frequency $\nu_{ex} \propto \sigma_{ex} v_T$ is much less than the frequency $\omega_n = T_n^{-1} \propto n^{-3}$ of a Rydberg electron and this imposes the restriction $n \lesssim 8.5\times 10^3$ $(n_i^{(0)}[\mathrm{cm}^{-3}])^{-1/7}(Z^3/T[\mathrm{eV}])^{1/14}$, which is numerically close to the condition (1). Therefore, if $n_i^{(0)} \sim 10^{14}\ \mathrm{cm}^{-3}$, the levels localized in the $Z = 1$ case are those with $n < 40$. It should be noted that in the case of an ideal plasma we have $r_s \ll r_D$ and, consequently, the orbit radius is much less than the Debye radius $r_n \ll r_D$. We shall assume that this condition is satisfied.

The equation for the equilibrium of charges of localized and free electrons is as follows (see Ref. 4):

$$r^{-1}(r\varphi)'' = 4\pi\,[n_e - Zn_i + |\psi_n|^2], \qquad (2)$$

where φ is the total potential, $n_i(r)$ and $n_e(r)$ are the concentrations of ions with a charge Z and of electrons in the continuous spectrum with energies $\varepsilon = p^2/2$ $(0 \lesssim \varepsilon < \infty)$, and $\psi_n(r)$ is the wave function of an electron of energy $\varepsilon_n < 0$ localized near the ion in question. We shall be interested in the situation when the quantities φ, n_i, and n_e in Eq. (2) are the values averaged over plasma fluctuations. Since n_i and n_e are nonlinear functions (see below) of the potential, it is clear that the replacement of the potential with the average value φ is justified for an equilibrium plasma when the energy of fluctuations is low compared with the thermal energy T, which is indeed true (see, for example, Ref. 10) for an ideal plasma, i.e., when the number of particles in a Debye sphere is high: $n_D = (4/3) n_e^{(0)} \pi r_D^3 \gg 1$. It should be noted that in this case the fluctuations of the concentrations of free charges n_e and n_i in the plasma are also small (they are proportional to $n_D^{-1/2}$), so that the use of equations for the determination of the average values n_e, n_i, and φ is statistically justified. Within the framework of the Debye model [i.e., when Eq. (2) is linearized] this problem is not encountered, because we can then assume that $(n_e - Zn_i) \propto \varphi$ and the average values of the concentrations can be determined rigorously in terms of the average values of the potential. However, this is one of the reasons why the Debye screening model is valid even when $n_D \ll 1$, as demonstrated recently in Ref. 11, where calculations were made by tracking many particles, allowing for the transient nature of the plasma microfield because of the motion of the plasma charges. The total potential φ is then close to the screened Coulomb potential if φ is understood to be the value averaged over a time t in which a Debye sphere contains many particles $[t \gg \tau_0 = (\pi r_D^2 N v_T)^{-1}]$. It should also be noted that the discussion given below applies only in the case of an equilibrium plasma characterized by $T_e = T_i$ and by the Maxwell–Boltzmann distributions of the particles. Otherwise it is necessary to allow for the effects of the dynamic polarizability of the plasma (see, for example, Ref. 12).

Using equilibrium distributions for free electrons with $\varepsilon > 0$ and a Boltzmann distribution for ions, we readily find that the densities n_e and n_i subject to the potential φ are described by

$$\begin{aligned} n_e(r) &= n_i^{(0)} Z \frac{2}{\pi^{1/2}} \int\limits_{(2\varphi)^{1/2}}^{\infty} \exp\left(-\frac{p^2}{2T} + \frac{\varphi}{T}\right) \frac{p^2\,dp}{2^{1/2} T^{3/2}} \\ &= Zn_i^{(0)} \left\{2\left(\frac{y}{\pi}\right)^{1/2} + (1 - \mathrm{erf}\,(y^{1/2})\,e^{y}\right\}, \\ n_i(r) &= n_i^{(0)} \exp(-Z\varphi/T), \end{aligned} \qquad (3)$$

where $y = \varphi/T$ and

$$\mathrm{erf}\,(x) = \frac{2}{\pi^{1/2}} \int\limits_0^x \exp(-x^2)\,dx$$

is the error function. The Debye screening model is applicable if the nonlinear relationships of Eq. (3) between the particle densities and the potential can be linearized, i.e., if $y = \varphi/T \ll 1$. Since to lowest order the potential at distances $r \sim r_n$ (of the order of size of the orbit of a quantum electron) is close to the Coulomb potential, the condition $y \ll 1$ sets an upper limit to the quantum number

$$n \geqslant 4Z/(T\ [\mathrm{eV}])^{1/2}. \qquad (4)$$

Thus, if $Z = 1$ and $T = 0.1$ eV, we find that $n \gtrsim 12$. It should be noted that linearization of Eq. (2) can be used also by way of estimate in the case of lower levels. This is due to the fact that the solutions of the linear and nonlinear equations should have the same asymptotes in the limit $r \to 0$. Moreover, these limits should be identical in the asymptotic range of large distances, where linearization is always justified. In the region $y = \varphi/T \ll 1$ allowing for Eq. (3), we readily obtain

$$n_e = Zn_i^{(0)}(1+y), \quad n_i(r) = n_i^{(0)}(1 - Zy).$$

The corresponding linearized equation is of the form

$$\begin{aligned} &r^{-1}(r\varphi)'' = 4\pi Z(Z+1)\,(\varphi/T)\,n_i^{(0)} + 4\pi\psi_n^2 = \lambda^2\varphi + 4\pi\psi_n^2, \\ &\varphi(r\to 0) = Z/r, \quad \varphi(r\to\infty) = (Z-1)/r, \end{aligned} \qquad (5)$$

where

$$\begin{aligned} &\lambda^2 = 1/r_D^2, \quad r_D = [T/4\pi n_i^{(0)} Z(Z+1)]^{1/2} \approx 1.4\cdot 10^{11} \\ &\cdot\{T\ [\mathrm{eV}]/[n_i^{(0)}[\mathrm{cm}^{-3}]\,Z(Z+1)]\}^{1/2}\ [\mathrm{a.u.}]. \end{aligned}$$

It should be noted that if we ignore the nonpoint nature of the charge of a bound electron [assuming in Eq. (5) that $\psi_n^2 = \delta(r)$], the solution of Eq. (5) is the screened Coulomb potential $(Z-1)e^{-\lambda r}/r$. The potential created by the medium can be found by subtracting from it the Coulomb potential $(Z-1)/r$ of the nucleus Z and the electron e^-, so that the polarization shift of hydrogen nl levels can be determined using perturbation theory:

$$\begin{aligned} \Delta E_{nl} &= \left\langle nl \left| -\frac{Z-1}{r} e^{-\lambda r} + \frac{Z-1}{r} \right| nl \right\rangle \approx (Z-1)\lambda\langle nl|nl\rangle \\ &- \frac{\lambda^2}{2}(Z-1)\langle r\rangle_{nl} = \frac{(Z-1)}{r_D} - \frac{3n^2 - l(l+1)}{4r_D^2}\,\frac{Z-1}{Z}. \end{aligned} \qquad (6)$$

Such an estimate of the shift of the levels was obtained in Ref. 7. We can see that all the nl levels are shifted by the same amount $\sim (Z-1)/r_D$ because of the arrival of free electrons at an ion and because of the screening of the field of the nucleus by these electrons. The experimentally observed shift of the $nl \to n'l'$ hydrogen lines is governed by the second term in Eq. (6), which is dependent on quantum numbers n and l and which is responsible for the stronger reduction in the level energies with higher values of n and a corresponding red shift of the lines. It is clear from Eq. (6) that the shift of the ionic lines is proportional to the charge density in the plasma and to the orbit size ($\propto n^2/r_D^2 \sim n_i^{(0)} n^2$), as confirmed by the experimental results given in Ref. 7. It should be noted that Eq. (6) is invalid when the nuclear charge Z is large. In particular, in the case of atoms it follows from Eq. (6) that the effects are canceled because of the action of the nuclear and bound electron charges on the medium, i.e, there is no shift.

3. CALCULATION OF THE POLARIZATION SHIFT USING A SELF-CONSISTENT DEBYE SCREENING MODEL

We shall introduce a screening function $\chi = r\varphi/Z$ for a charge Z in a plasma. Applying the linearized model of Eq. (5), we obtain the following equation and the relevant boundary conditions needed to determine this function:

$$\chi'' = \lambda^2 \chi + R_{nl}^2/Zr, \quad \chi(0) = 1, \quad \chi(\infty) = 0. \tag{7}$$

In the zeroth approximation we can regard the wave function $\psi_{nl} = (R_{nl}/r) Y_{lm}$ of a quantum electron close to the Coulomb function of a hydrogen-like ion. In the derivation of Eq. (7) the density of a quantum electron in an nl state is averaged over the magnetic quantum numbers using the expression

$$(2l+1)^{-1} \sum_{m=-l}^{l} (R_{nl}^2 Y_{lm}/r^2) = R_{nl}^2/4\pi r^2.$$

The solution of the linear equation (7) with a given function R_{nl}^2/Zr is readily obtained by, for example, the method of variation of constants:

$$\chi(r) = e^{-\lambda r}\left(1 - \int_0^r dx \frac{R_{nl}^2}{Zx} \frac{e^{\lambda x} - e^{-\lambda x}}{2\lambda}\right) - \frac{e^{\lambda r} - e^{-\lambda r}}{2\lambda} \int_r^\infty dx \frac{R_{nl}^2}{Zx} e^{-\lambda x}. \tag{8}$$

Clearly, the functions $\exp(\pm\lambda x)$ vary slowly (because of the condition $r_n \ll r_D = 1/\lambda$) compared with the function R_{nl}^2/x in the region of the quantum electron orbit. Consequently, using expansion as a series

$$\exp(\pm\lambda x) = 1 \pm \lambda x + \lambda^2 x^2/2 + \ldots,$$

we can obtain the asymptotic solution of Eq. (8):

$$\chi = \frac{Z-1}{Z}\left(1 - \lambda r + \frac{1}{2}\lambda^2 r^2\right) + \frac{1}{Z}\int_r^\infty dx\, R^2\left(1 - \frac{r}{x}\right) + \frac{1}{2}\frac{\lambda^2 r^2}{Z}\left[\int_r^\infty dx\, R^2\left(1 - \frac{x}{r}\right) - \frac{1}{3}\int_0^r dx \frac{x^2}{r^2} R^2 - \frac{1}{3}\int_r^\infty dx\, R^2 \frac{r}{x}\right]. \tag{9}$$

In view of the linearity of Eq. (7), the total potential φ can be represented by the following sum:

$$\varphi = V_e + \frac{Z}{r} + V_p, \quad V_e = -\frac{1}{r} + \frac{1}{r}\int_r^\infty \left(1 - \frac{r}{x}\right) R^2\, dx, \tag{10}$$

where V_e is the potential created by a quantum electron, Z/r is the Coulomb potential of the nucleus, V_p is the potential of the medium created by ions and free electrons in the plasma, i.e.,

$$V_p = -\int \frac{n_e(\mathbf{r}') - Zn_i}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \approx -\lambda^2 \int \frac{\varphi(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'.$$

Using Eq. (10) for the potential created by a plasma in the region of a quantum electron, we readily obtain

$$V_p = -(Z-1)\lambda + \frac{1}{2}\lambda^2 r(Z-1) - \frac{1}{2}\lambda^2 r\left[\int_r^\infty dx\, R^2\left(\frac{x}{r} - 1\right) + \frac{1}{3r^2}\int_0^r x^2 R^2\, dx + \frac{r}{3}\int_r^\infty \frac{R^2}{x} dx\right]. \tag{11}$$

It is this potential ($-V_p$) that determines the energy of the polarization shift of the levels, i.e., $\Delta E_{nl} = -\langle nl | V_p | nl \rangle$. We can see that the shift due to the first two terms in Eq. (11) is governed by the reaction of the medium to the system formed by a nucleus Z and an electron, which are located at the same point ($r = 0$). This shift is naturally given by Eq. (6). The third term in Eq. (11) is negative and it appears because of the spatial distribution of the charge of a quantum electron, which results in a stronger screening due to the additional inflow of free electrons to the center. The binding energy of a quantum electron then decreases.

We shall first consider the polarization shift of high levels $n \gg 1$ characterized by small values of the orbital momentum $l \ll n$. In this case it is natural to describe R_{nl} quasiclassical wave functions

$$R_{nl} \approx \left(\frac{2}{\pi n^3}\right)^{1/2} \frac{1}{(k_r)^{1/2}} \cos\left(\int^r k_r\, dr - \frac{\pi}{4}\right),$$

where $k_r = (Z/r - Z^2/2n^2)^{1/2}$ is the radial wave vector. Averaging over oscillations of the wave function gives

$$R_{nl}^2 = \frac{2Z^2}{\pi n^3}\left(\frac{2Z}{r} - \frac{Z^2}{n^2}\right)^{-1/2} \overline{\cos^2}\left(\int^r k_r\, dr - \frac{\pi}{4}\right) \approx \frac{Z^2}{\pi n^2}\left(\frac{2n^2}{Zr} - 1\right)^{-1/2}. \tag{12}$$

Substituting this expression in Eq. (11) and applying perturbation theory to determine the polarization shift (i.e., $\Delta E_{nl} = -\langle nl | V_p | nl \rangle$), we obtain

$$\Delta E_{nl} = \Delta E_{nl}^{(1)} + \Delta E_{nl}^{(2)} + \Delta E_{nl}^{(3)},$$

where

$$\Delta E_{nl}^{(1)} = (Z-1)\lambda \langle nl | nl \rangle = (Z-1)/r_D, \tag{13a}$$

$$\Delta E_{nl}^{(2)} = -\frac{2}{\pi}\frac{\lambda^2 n^2}{Z}(Z-1)\int_0^1 dr_0\, r_0^{3/2}(1-r_0)^{-1/2} = -\frac{2}{\pi}\frac{\lambda^2 n^2}{Z}(Z-1) B\left(\frac{5}{2}, \frac{1}{2}\right) = -\frac{3}{4}\frac{(Z-1)}{Z}\frac{r_n}{r_D^2}, \tag{13b}$$

$$\Delta E_{nl}^{(3)}=\frac{4}{\pi^2}\frac{\lambda^2n^2}{Z}J,\qquad J=\int\limits_0^1 dr_0 r_0^{3/2}(1-r_0)^{-1/2}$$

$$\cdot\left[\int\limits_{r_0}^1 dx x^{1/2}(1-x)^{-1/2}\left(\frac{x}{r_0}-1\right)+\frac{1}{3r_0^2}\int\limits_0^{r_0} dx x^{5/2}(1-x)^{-1/2}\right.$$

$$\left.+\frac{r_0}{3}\int\limits_{r_0}^1 dx x^{-1/2}(1-x)^{-1/2}\right]. \qquad (13c)$$

Here, $B(\alpha,\beta)$ is the beta function and $\Delta E_{nl}^{(i)}$ corresponds to the contribution made to the polarization shift by the three terms in Eq. (11). As expected, the first two are exactly identical with Eq. (6), i.e., the use of semiclassical functions introduces no error. Less trivial is the calculation of the integrals in Eq. (13c). Altering the order of integration in the first of the integrals in Eq. (13c) and applying integration by parts, we can obtain

$$J=B\left(\frac{5}{2},\frac{1}{2}\right)B\left(\frac{3}{2},\frac{1}{2}\right)-2J_1+\frac{2}{3}J_2=\frac{3\pi^2}{16}+\frac{2}{3}J_2-2J_1, \qquad (14)$$

$$J_2=B\left(\frac{7}{2},\frac{1}{2}\right)\int\limits_0^1 dt t^{-1/2}(1-t)^{-1/2}I_t\left(\frac{7}{2},\frac{1}{2}\right),$$

$$J_1=B\left(\frac{5}{2},\frac{1}{2}\right)\int\limits_0^1 dt t^{1/2}(1-t)^{-1/2}I_t\left(\frac{5}{2},\frac{1}{2}\right).$$

Using the recurrence relationship[13] for a partial beta function

$$I_t(\alpha,\beta)=tI_t(\alpha-1,\beta)+(1-t)I_t(\alpha,\beta-1)$$

and integrating the integrals in Eq. (14) by parts, we find that certain operations yield the relationships

$$J_2=\frac{5}{3}J_1-\frac{2}{3},\qquad J_1=\frac{3\pi^2}{32}-\frac{1}{6}.$$

Using these relationships, we obtain the polarization shift $\Delta E_{nl}^{(3)}$ due to the spatial nonpoint nature of a quantum electron

$$\Delta E_{nl}^{(3)}=\frac{4}{\pi^2}\frac{\lambda^2n^2}{Z}J=\frac{4}{\pi^2}\frac{\lambda^2n^2}{Z}\left(\frac{5\pi^2}{48}-\frac{8}{27}\right)$$

$$\approx 0.3\frac{\lambda^2n^2}{Z}=0.2\frac{r_n}{r_D^2},$$

$$\Delta E_{nl}=\Delta E_{nl}^{(1)}+\Delta E_{nl}^{(2)}+\Delta E_{nl}^{(3)}$$

$$=(Z-1)\lambda-\frac{\lambda^2n^2}{Z}\left[\frac{3}{4}(Z-1)-0.3\right]. \qquad (15)$$

Therefore, all the levels experience the same shift $\Delta E_{nl}^{(1)}=\lambda(Z-1)$ independent of n as well as a shift dependent on n, which governs the polarization shift of the lines:

$$\Delta E_{nl}^{(2)}+\Delta E_{nl}^{(3)}=(\lambda^2n^2/Z)\,[0{,}3-{}^3/_4(Z-1)\,].$$

In the case when $Z=1$, we obtain $\Delta E_{nl}^{(2)}+\Delta E_{nl}^{(3)}=0.3\lambda^2n^2$, for $Z=2$ we find that $\to -0.23\lambda^2n^2$, for $Z=3$ we have $\to -0.4\lambda^2n^2$, and for $Z\to\infty$ the result $\to -0.75\lambda^2n^2$ is identical with that given by the model of Ref. 7. We can see that in the case of hydrogen with $Z=1$ the n-dependent shift results in the level expansion, in contrast to the case of ions with $Z>1$ when the binding energy of the levels increases. The corresponding spectral lines of the hydrogen atom experience a "blue" (and not red, as in the case of ions) polarization shift. The magnitude of the effect is even greater than for He II ions, but the resultant direction of the shift for H I is governed by competition with the quadrupole Stark shift.[7-9]

We shall now consider the case when $l\sim n$. The orbits of a quantum electron are then close to a circle of radius $r\sim r_0=n^2$. Expanding the Coulomb wave function as a series at a stationary point, we obtain

$$R_{n,l=n-1}^2=\frac{(2r)^{2n}e^{-2r/n}F(0,2n,2r/n)}{n^{2n+1}(2n-1)!}$$

$$\approx\frac{\exp(2n-4n\ln n+2n\ln r-2r/n)}{(\pi n)^{1/2}}$$

$$\approx\frac{\exp\{-(r-n^2)^2/n\}}{(\pi n)^{1/2}}. \qquad (16)$$

Clearly, in the case of sufficiently large values of n this function is close to the δ function, which corresponds to a circular orbit. We shall therefore assume that $R^2\approx\delta(r-n^2/Z)$ for an ion with a charge Z. This approximation allows us to calculate readily the integrals in Eq. (11). The nonpoint part of the potential of the medium and the polarization shift are then described by

$$V_p^{(3)}=-\frac{1}{2}\lambda^2r\left[\left(\frac{n^2}{Zr}-1\right)+\frac{1}{3}\frac{Zr}{n^2}\right]\quad\text{for}\quad r<\frac{n^2}{Z},$$

$$V_p^{(3)}=-\frac{1}{6}\frac{\lambda^2n^4}{rZ^2}\quad\text{for}\quad r>\frac{n^2}{Z} \qquad (17)$$

and, correspondingly,

$$\Delta E_{nl}=(Z-1)\lambda-\frac{1}{2}\frac{\lambda^2n^2}{Z}\left[\frac{3}{2}(Z-1)-\frac{1}{3}\right]. \qquad (18)$$

We can see that for $Z\gg1$, this result is identical with both Eqs. (15) and (6), because in this case the nonpoint nature of a quantum electron is unimportant. If $Z=1$, the n-dependent shift of the levels with $l\ll n$ is approximately twice that in the case when $l\sim n$. This is due to the fact that the electron charge is shifted away from the center further in the case of elongated orbits, so that the average orbit size $\langle r\rangle_{nl}\sim 3n^2/2Z$ in the $l\ll n$ case exceeds $\langle r\rangle_{nl}\sim n^2/Z$ in the case when $l\sim n$.

4. NONLINEAR MODEL OF SELF-CONSISTENT SCREENING AND DISCUSSION OF RESULTS

We shall now analyze the numerical solution of the nonlinear equation (2). Using the expressions in Eq. (3) and introducing dimensionless parameters

$$T_0=Tr_n,\qquad n_0=n_i^{(0)}r_n^3,\qquad \lambda_0^2=\left(\frac{r_n}{r_D}\right)^2=\frac{4\pi Z(1+Z)n_0}{T_0}, \qquad (19)$$

we can rewrite Eq. (2) in a more convenient form

$$\frac{d^2}{dr_0^2}\chi_p=n_0r_0\left[2\left(\frac{y}{\pi}\right)^{1/2}+(1-\mathrm{erf}(y^{1/2}))e^y-e^{-zy}\right]. \qquad (20)$$

The following notation is used above:

$$r_n=2n^2/Z, \quad r_0=r/r_n, \quad y=Z\chi/Tr=Z(\chi_0+\chi_p)/T_0r_0,$$

where the screening functions χ_0 and χ_p are introduced in such a way that the potential $\varphi_0=Z_{\chi_0}/r$ corresponds to the potential created by a nuclear charge and a quantum electron (i.e., $\Delta\varphi_0=4\pi\psi_n^2$), whereas $\varphi_p=Z_{\chi p}/r$ corresponds to the potential created by plasma charges. It should be pointed out that, in accordance with Eq. (10), the screening function χ_0 is described by the expression

$$\chi_0=\frac{Z-1}{Z}+\frac{1}{Z}\int_r^\infty\left(1-\frac{r}{x}\right)R^2\,dx. \qquad (21)$$

Note that the potential φ (and, consequently, the function χ) should show reversal of the sign in the case of screening of the hydrogen atom, i.e., when $Z=1$. In fact, multiplying Eq. (2) by r^2, integrating with respect to dr from 0 to ∞, and allowing for the boundary conditions and the normalization of the wave function of a quantum electron, we readily obtain the following relationship:

$$\int_V d\mathbf{r}[n_e(\mathbf{r})-Zn_i(\mathbf{r})]=Z-1. \qquad (22)$$

It follows from this relationship that in the case of screening of neutral atoms the total charge of free electrons reaching an atom from infinity is zero (in contrast to the screening of ions when we have $Z\geqslant 2$), i.e., there is only polarization of the plasma and free electrons expelled by a quantum electron are displaced toward the ion core. Clearly, this behavior of the plasma charges is possible only if the total potential φ has a variable sign, because the excess of electrons in the region of a nucleus corresponds to $\varphi>0$, and a deficiency in another region corresponds to $\varphi<0$. The expressions in Eq. (3) are not valid for $\varphi<0$, but—as demonstrated by the solutions given below—in the region $\varphi\lesssim 0$ we can accurately use a linearized model of Eq. (7), which is valid for any signs of the potential φ if $y=\varphi/T\ll 1$. Equation (20) is then of the form

$$\frac{d^2}{dr_0^2}\chi_p=\lambda_0^2(\chi_0+\chi_p). \qquad (23)$$

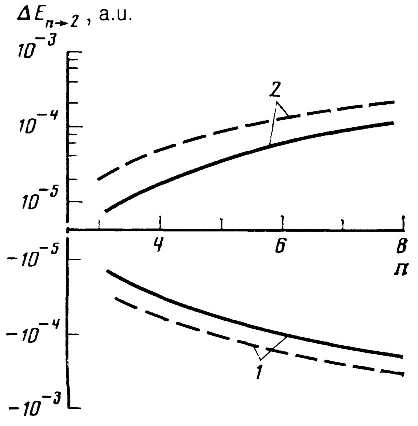

FIG. 1. Energy shift of the lines due to $n\to 2$ transitions for H I atoms (curve 1) and He II ions (curve 2). The dashed curves are calculated on the basis of Eq. (15) and the continuous ones represent numerical calculations based on the nonlinear screening model ($T=1$ eV, $r_D=250a_0$).

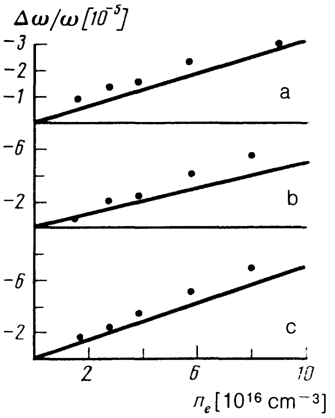

FIG. 2. Dependence of the relative shift of the 4→3 (a), 5→3 (b), and 6→3 (c) lines of He II ions on the electron concentration $n_e^{(0)}$ in a plasma ($T=4$ eV). The continuous lines are calculated using Eq. (24) allowing for estimates[7] of the contribution of the quadrupole Stark effect. The points are the experimental values.[7]

Therefore, in the numerical calculations a start is made at $r=0$ using the solution of the nonlinear equation (20) and in the region $y=\varphi/T\ll 1$ (i.e., in the asymptote of the solution) this equation is replaced with the equivalent—in this range—Eq. (23).

The results of calculations of the polarization shift for the $n\to 2$ ($n=3$–8) transitions in H I and He II, carried out using the framework of the nonlinear screening of Eq. (20), are compared in Fig. 1 with those obtained using analytic expressions of Eq. (15) in the linearized model.

It follows from Eq. (4) that the linearized model is valid for $n\geqslant 4$ and $n\geqslant 6$ for the cases $Z=1$ and $Z=2$, respectively. It is clear from Fig. 1 that the error of the linearized model amounts to more than 100% at $n=3$, that it decreases on increase in n and that where the linear model is valid it is less than 30–40%. Therefore, we can draw the conclusion that Eqs. (15) and (18), obtained, give satisfactory results in a self-consistent Debye model of the polarization shift in the range where the condition (4) is obeyed.

Under the experimental conditions of Ref. 7, when $n=4, 5, 6\to n'=3$, $Z=2$, and $T=4$ eV, the condition (4) is satisfied if $n\gtrsim 3$. Consequently, if we use Eqs. (15) and (18) to average approximately over l and l', we find that the

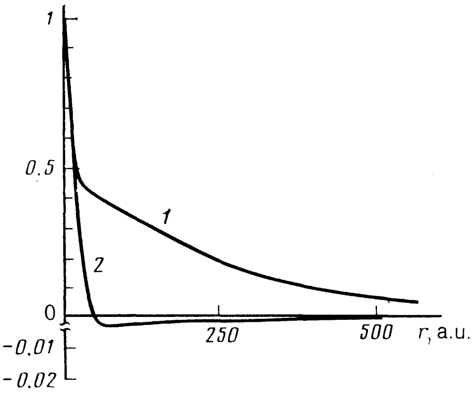

FIG. 3. Screening function χ of the total potential for He II ions (curve 1) and He I atoms (curve 2).

relative shift $\Delta\omega/\omega_0$ of the lines for the $n \rightarrow n'$ transition is

$$\frac{\Delta\omega}{\omega_0} \approx -\frac{3(Z-1)/2-0{,}47}{Z}\left(\frac{nn'}{Zr_D}\right)^2 . \tag{24}$$

It is clear from Fig. 2 that the values of the relative shift $\Delta\omega/\omega_0$ calculated using this expression for different $n \rightarrow n'$ transitions agree well with the corresponding experimental results. Estimates of the short-wavelength shift due to the quadrupole Stark effect in the case of ions, obtained in Ref. 7 on the basis of the theory of Refs. 8 and 9 for given plasma parameters, give values smaller than the corresponding polarization shifts. We can therefore assume that the experimentally observed red shift of the lines is due to the polarization effect.

Figure 3 shows the screening functions for the total self-consistent potential φ in the case of the hydrogen atoms H I and helium ions He II, obtained by numerical solution of Eq. (20). As expected, the potential in the $Z = 1$ case has variable sign. We can see also that in the region of the minimum of the potential at $r \sim r_{\min} = (70\text{–}80)a_0$ the linearization of Eq. (2) is justified, because we then have $\varphi(r_{\min})/T \sim 2 \times 10^{-3} \ll 1$. It should be also pointed out that the point r_0^*, at which $\varphi(r_0^*) = 0$, separates the region of a positive charge from a negatively charged region $r > r_0$. The kink in the curve $\chi(r)$ for the $Z = 2$ case observed at $r \gtrsim r_n = 25a_0$ is related to the change in the screening regime, because for $r < r_n$ the screening is mainly due to a quantum electron, whereas for $r > r_n$ it is due to free charges in a plasma.

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