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New Source of the Red Shift of Highly-Excited Hydrogenic Spectral Lines in Astrophysical and Laboratory Plasmas

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Abstract

High-n hydrogen spectral lines (SL), n=13–17, studied in astrophysical and laboratory observations at the electron density $N_e \sim 10^{13}$ cm^{-3} by Bengtson and Chester in 1972 (ApJ, p. 178, 565) exhibited red shifts by orders of magnitude greater than the theoretical shifts known up to now. Specifically, Bengtson and Chester presented the shifts of these SL observed in the spectra from Sirius and in the spectra from a radiofrequency discharge plasma in the laboratory: both types of the observations yielded red shifts that exceeded the corresponding theoretical shifts by orders of magnitude. In the present paper we introduce an additional source of the shift of high-n hydrogenic SL. We show that for high-n hydrogen SL it makes the primary contribution to the total red shift. We demonstrate that for the conditions of the astrophysical and laboratory observations from paper by Bengtson and Chester, this additional red shift is by orders of magnitude greater than the theoretical shifts known up to now. Finally we show that the allowance for this additional red shift removes the existed huge discrepancy between the observed and theoretical shifts of those that of high-n hydrogen SL.

Keywords: Astrophysical plasmas; Shifts of hydrogen spectral lines; Measurements; Red shift; Laboratory plasmas

Introduction

Spectral lines (hereafter, SL) of hydrogenic atoms/ions in plasmas are typically red-shifted by electric microfields by microfields – see, e.g., books by Griem [1] and Oks [2]. This Stark shift is important not only fundamentally, but also practically. In astrophysics, red shifts of SL are observed in various astrophysical objects: for deducing the relativistic (cosmological and gravitational) red shifts (see, e.g., book by Nussbaumer and Bieri [3]) from observed red shifts it is necessary to take into account the Stark shift. In laboratory plasma diagnostics, measurements of the Stark shift can complement measurements of the Stark width for determining the electron density – see, e.g., paper by Parigger et al. [4].

The best studied are shifts of hydrogen SL (especially of the H-alpha line). For low-n hydrogen SL (n being the principal quantum number of the upper level), studied experimentally mostly at the electron densities $N_e=10^{16}–10^{19}$ cm^{-3} and slightly higher, in the course of time there was achieved an agreement between the experimental and theoretical shifts – see, e.g., books by Griem [1] and Oks [2], as well as papers by Grabowski and Halenka [5], Demura et al. [6], Demura et al. [7], Djurovic et al. [8], Kielkopf and Allard [9] and references therein.

However, high-n hydrogen SL (n=13–17), studied in astrophysical and laboratory observations at $N_e \sim 10^{13}$ cm^{-3} by Bengtson and Chester [10], exhibited red shifts by orders of magnitude greater than the theoretical shifts known at that time (in 1972) or at any later time up to now. Specifically, in paper by Bengtson and Chester [10] there were presented the shifts of these SL observed in the spectra from Sirius and in the spectra from a radiofrequency discharge plasma in the laboratory: both types of the observations yielded red shifts that exceeded the corresponding theoretical shifts by orders of magnitude. In the same year Barcza [11] presented observations of hydrogen SL of n=19-23 in the spectrum from Sirius, i.e., higher-n SL than observed in the spectra from Sirius by Bengtson and Chester [10]. In a later paper Barcza [12] wrote “measurements in the spectrum of Sirius Barcza [11] did not show any shift of Balmer lines lower than H21” and questioned the shifts observed in the spectra from Sirius by Bengtson and Chester [10]. However, first Barcza [11] did not observe the same SL as Bengtson and Chester [10]. Rather, Barcza [11] observed higher SL (n=19–23) than SL of n=13–17 observed in the spectra from Sirius by Bengtson and Chester [10]. As the principal quantum number n increases, the SL become much weaker in their absolute intensity, and also become much broader and thus subjected to blending/merging with adjacent SL. (In paper by Barcza [11] the author himself noted that the observed lines H20 and H21 were subjected to blending.) For these reasons it is much more difficult to reliably measure shifts of such higher-n SL observed by Barcza [11]. In distinction, Bengtson and Chester [10] emphasized that in their observations “no measurements of the profile center were taken where there was strong blending in the wings”. Thus, in reality observations by Barcza [11] in the spectrum of Sirius do not disprove observations by Bengtson and Chester [10] in the spectra of Sirius.

As for further observations of shifts of high-n hydrogen SL in laboratory plasmas in the same range of n as in paper by Bengtson and Chester [10], such an experiment was reported by Himmel [13] who observed hydrogen SL of n=12–19. The comparison with the shifts of hydrogen SL of n=13–17 observed in the laboratory plasma by Bengtson and Chester [10] had shown the following. The shifts of SL H13, H14, and H16 agreed in these two experiments within the error margins, but the shift of SL H15 and H17 observed by Himmel [13] were significantly smaller than the corresponding shifts observed by Bengtson and Chester [10] and Himmel [13] suggested that the larger shifts measured by Bengtson and Chester [10] “are caused by some kind of systematic error … as far as the investigation of the laboratory plasma is concerned”. However, first Himmel [13] emphasized that “direct comparison of observations is not possible because different plasma parameters were used”. Second, it seems inconsistent to assume that in the laboratory measurements by Bengtson and Chester [10], two

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SL (H15 and H17) were subjected to a some kind of systematic error, while three other SL (H13, H14, and H16) were in agreement with the shift measurements by Himmel [13] and thus were not subjected to the same systematic error. Third, measurements of the widths of the high-n hydrogen SL by Himmel [13] versus n showed that in the range of n=12–17 the width increased with the growing n, but in the range of n=17–19 the width decreased with growing n by Himmel [13]. The decrease of the width with the growing n in the range of n=17–19 contradicts to any modern theory of the Stark broadening of hydrogen SL and thus could indicate some systematic error in the experiment by Himmel [13].

Let us summarize the above situation–first for the astrophysical observations and then for the laboratory observations:

1. In the spectra of Sirius, the relatively large, theoretically unexplained shifts of the high-n hydrogen SL in the range of n=13–17, observed by Bengtson and Chester [10] actually have not been disproved by Barcza [11,12] who observed significantly higher-n hydrogen SL (n =19–23) that are much weaker, broader and thus subject to blending (making them less reliable) compared to the SL of n=13–17 observed by Bengtson and Chester [10]. In other words Barcza [11,12] compared "apples with oranges" instead of comparing "apples with apples".

2. The two laboratory experiments on the shifts of high-n hydrogen SL - by Bengtson and Chester [10] and by Himmel [13]–agreed with each other (within the error margins) with respect to 3 out 5 SL measured by Bengtson and Chester [10]and disagreed with respect to 2 out 5 SL measured by Bengtson and Chester [10]. However, plasma parameters in the two experiments differ from each other and Himmel [13] emphasized that the direct comparison was not possible. Besides, the dependence of widths of the high-n hydrogen SL measured by Himmel [13] on n contradicts to the modern Stark broadening theories and could be symptomatic of a systematic error.

3. Himmel [13] wrote that "it seems desirable to determine which theoretical model if any qualifies for explaining detectable line shifts" of these high-n hydrogen SL as studied by Himmel [13]. Up to now there was no theoretical explanation of the relatively large, detectable line shifts of high-n hydrogen SL observed in the spectra of Sirius and in the spectra from the corresponding laboratory plasma. So, there is still the need for such explanation.

In the present paper we introduce an additional source of the shift of high-n hydrogenic SL. We show that for high-n hydrogen SL it makes the primary contribution to the total red shift. We demonstrate that for the conditions of the astrophysical and laboratory observations from paper by Bengtson and Chester [10], this additional red shift is by orders of magnitude greater than the theoretical shifts known up to now (below we refer to the latter as the "standard shifts"). Further we show that the allowance for this additional red shift leads to the agreement with the astrophysical red shifts for all four high-n hydrogen SL observed in paper by Bengtson and Chester [10] and to the agreement with the laboratory red shifts, for four out of five high-n hydrogen SL observed in the same paper. The last but not least–the theory developed in the present paper has the fundamental importance in its own right: it can be applied also to the high-n SL of hydrogen like ions and thus motivate further observations of the shifts of not only hydrogen SL, but also of SL of hydrogen like ions.

n	λn (A)	Se (A)	S_{Sirius} (A)	S_{exp} (A)
13	3734	0.0017	--	0.03 ± 0.03
14	3722	0.0021	0.03 ± 0.05	0.00 ± 0.04
15	3712	0.0026	0.09 ± 0.07	0.15 ± 0.05
16	3704	0.0032	–0.007 ± 0.05	0.00 ± 0.05
17	3697	0.0038	0.21 ± 0.08	0.30 ± 0.08

Table 1: Electronic shift Se of the hydrogen spectral lines H13 – H17, calculated by formulas from papers by Griem [14,16] and their comparison with the shifts from paper by Bengtson and Chester [10].

"Standard" Shifts of High-n Hydrogen Lines and their Comparison with Observations

For the electron densities $N_e \sim 10^{13}$ cm^{-3}, there are the following two major "standard" contributions to the shift of high-n hydrogen SL–in order of diminishing magnitude. The largest standard contribution is due to quenching, i.e., non-zero Δn (Griem [14]) and elastic, i.e., zero Δn (Boercker and Iglesias [15]) collisions with plasma electrons–hereafter, the electronic shift (see also paper by Griem HR [16]). For high-n lines, the primary component of the electronic shift comes from the quenching collisions: it scales as $\sim n^4$, while the secondary component (originating from the elastic collisions) scales as $\sim n^2$.

Table 1 presents the electronic shift Se of the hydrogen SL H_{13}–H_{17}, calculated by formulas from papers by Griem [14,16], and their comparison with the shifts from paper by Bengtson and Chester [10] observed in astrophysical and laboratory plasmas. It is seen that the electronic shift is by orders of magnitude smaller than both the shift of the SL H_{14}, H_{15}, H_{17} observed in the spectrum of Sirius and the shift of the SL H_{13}, H_{15}, and H_{17} observed in the laboratory plasma.

This comparison already shows the inability to explain the observed shifts from paper by Bengtson and Chester [10] by the "standard" sources of the shift. This is because the second largest "standard" shift is by one or even two orders of magnitude smaller than the first "standard" shift (the electronic shift). For this reason it is sufficient to estimate the second largest standard shift just by the order of magnitude, as we do below.

Specifically, by evaluating the second largest standard shift we mean the standard approach to calculate the contribution to the shift from plasma ions–hereafter, the standard ionic shift.

For the parameters relevant to the laboratory experiment from paper by Bengtson and Chester [10] (n=13–17, N_e=1.2 × 10^{13} cm^{-3}, T=2000 K) and the similar parameters for the astrophysical observations from the same paper, the ions can be considered quasistatic. In the standard approach the first step in calculating the contribution of the ionic shift is to use the multipole expansion with respect to the ratio r_{rms}/R (in the binary description of the ion microfield) or with respect to the analogous parameter $r_{rms}F^{1/2}$ (in the multi-particle description of the ion microfield F), where r_{rms} is the root-mean-square value of the radius-vector of the atomic electron ($r_{rms} \sim n^2/Z_1$, where Z_1 is the nuclear charge), and R is the separation between the nucleus of the radiating atom/ion and the nearest perturbing ion. Here and below we use the atomic units.

It was quite obvious that the dipole term of the expansion ($\sim 1/R^2$ or $\sim F$) does not lead to any shift of a hydrogenic SL. This is because each pair of the Stark components, characterized by the electric quantum numbers q and –q, is symmetric with respect to the unperturbed frequency ω_0 of the hydrogenic line–in terms of both the displacement from ω_0 and the intensity. (Here $q=n_1-n_2$, where $n_1$and n_2 are the first two of the three parabolic quantum numbers (n_1n_2 m).) As for the quadrupole term of the expansion ($\sim 1/R^3$ or $\sim F^{3/2}$), it does not shift the center of gravity of hydrogenic lines, as rigorously proven analytically in paper Oks [17]. Namely, after taking into account the quadrupole corrections not only to the energies/frequencies, but also to the intensities, and then summing up over all Stark components of a hydrogenic SL, the center of gravity shift vanishes at any fixed value of R or F_1 [18]. So, within the approach of the multipole expansion, the first non-vanishing ionic contribution to the shift of hydrogenic SL should come from the next term of the multipole expansion: from the term ~ $1/R^4$ or ~ F^2. While considering this term, some authors limited themselves by the quadratic Stark (QS) effect (such as, e.g., in papers by Griem HR [16, 18, 19]):

$$\Delta E_{QS}^{(4)} = -[Z_2^2 n^4 / (16 Z_1^4 R^4)]\,(17n^2 - 3q^2 - 9m^2 + 19) \qquad (1)$$

where Z_2 is the charge of perturbing ions; the superscript (4) at ΔE_{QS} indicates that this term is of the 4^{th} order with respect to the small parameter r_{rms}/R. Here and below we use the atomic units $\hbar = e = m_e = 1$, unless specified to the contrary.

However, first, it is inconsistent to take into account the quadratic Stark corrections to energies, but not to the intensities of Stark components (as in papers by Könies and Günter [19,20]). The corrections to the energies are of the same order as the corrections to the intensities, as noted in paper by Demura et al. [6]. Second, the following deficiency of papers by Griem [16], by Könies and Günter [19,20]): is even more important with regard to the energy correction of the order ~ $1/R^4$. The above Equation (1) originated from the dipole term (of the multipole expansion) treated in the 2nd order of the perturbation theory. However, the quadrupole term, treated in the 2^{nd} order of the perturbation theory, and the octupole term, treated in the 1^{st} order of the perturbation theory, actually also yield energy corrections ~ $1/R^4$, as it was shown as yearly as in 1969 by Sholin [21]. The rigorous energy correction of the order ~ $1/R^4$ has the form (as in 1969 by Sholin [21] and presented also in book Komarov et al. [22]):

$$\begin{aligned}\Delta E^{(4)} &= [Z_2\, n^3 / (16 Z_1^4 R^4)] \\ &[Z_1\, q(109q^2 - 39n^2 - 9m^2 + 59) - Z_2\, n(17n^2 - 3q^2 - 9m^2 + 19)]\end{aligned} \qquad (2)$$

Obviously, it is inconsistent to allow for one term and to neglect two other terms of the same order of magnitude.

For our purpose, it is sufficient to evaluate the standard ionic shift contribution by calculating the multipole corrections only to the energies–for three reasons. First, the ionic shift contribution caused by the corresponding multipole corrections to the intensities of the Stark components of a hydrogen line are of the same order of magnitude as ionic shift contribution caused by the multipole corrections to the energies. Second, frequently there is a partial cancellation of these two sources of the standard ionic shift: multipole corrections to the intensities of the Stark components frequently result in the shift to the opposite direction compared to the shift contribution caused by the multipole corrections to the energies, as noted in paper by Demura et al. [6]. Third, the calculations will show that the total standard ionic shift is several times smaller than the electronic shift, so that evaluating the former by the order of magnitude would be adequate.

While calculating the ionic multipole corrections only to the energies, we took into account not only the rigorous expression for the term $\Delta E^{(4)} = \sim 1/R^4$ given by Equation (2), but also the rigorous analytical expressions for the terms $\Delta E^{(5)} \sim 1/R^5$ and $\Delta E^{(6)} \sim 1/R^6$ presented in book by Komarov et al. [22] in Equation (4.59). Specifically for the parameters corresponding to the observations from paper by Bengtson and Chester [10] ($N_e = 1.2 \times 10^{13}$ cm^{-3}, $Z_1 = Z_2 = 1$), the results are shown in Table 2 in the column $S_{i,\,standard}$.

It is seen that the total standard ionic shift $S_{i,\,standard}$ is indeed several times smaller than the electronic shift S_e. Thus, regardless of whether or not the calculations of $S_{i,\,standard}$ would include also corrections to the intensities of the Stark components, $S_{i,\,standard}$ would remain a relatively small addition to S_e and the huge discrepancy with the observed shifts from paper Bengtson and Chester [10] would remain unexplained. So, while introducing below a new source of the red shift, which is by orders of magnitude greater than S_e, we then compare the observed shifts from paper Bengtson and Chester [10] just with the sum of the new shift and S_e, while $S_{i,\,standard}$ will be included in the theoretical estimate of the error margins of the final results. We also note that the so-called "plasma polarization shift", which plays an important role in explaining the observed shifts of the high-n SL of hydrogenic ions, was found in paper by Theimer and Kepple [23] to be negligibly small for the high-n SL of hydrogen atoms.

New Source of the Red Shift of High-N Hydrogenic Lines and the Comparison of the Total Theoretical Shift with Observations

The standard approaches to calculating the ionic contribution to the shift of hydrogenic SL, discussed in the previous section, used the multipole expansion in terms of the parameter r_{rms}/R that was considered small. All terms of the multipole expansion, starting from the quadrupole term, at the averaging over the distribution of the separation R between the nucleus of the radiating atom/ion and the nearest perturbing ion, led to integrals diverging at small R. These diverging integrals were evaluated one way or another, e.g., by introducing cutoffs. However, the mere fact that the integrals were diverging, was an indication that the standard approach did not provide a consistent complete description of the ionic contribution to the shift. The fact is that the standard approaches disregarded configurations where $r_{rms}/R > 1$, i.e., where the nearest perturbing ion is within the radiating atom/ion (below we call them "penetrating configurations"). For low-n hydrogenic SL, the statistical weight of penetrating configurations is relatively small, but it rapidly increases with n approximately ~ n^6.

For penetrating configurations, it is appropriate to use the expansion in terms of the parameter $R/r_{rms} < 1$ in the basis of the spherical wave functions of the so-called "united atom", which is a hydrogenic ion of the nuclear charge Z_1+Z_2. The energy expansion has the form e.g., book by Komarov et al. [22] Equation (5.10 - 5.12)):

$$E = -(Z_1 + Z_2)^2 / (2n^2) + O(R^2 / r_{rms}^{\ 2}) \qquad (3)$$

[1]We note in passing paper by Caby-Eyraud et al. [18] focused at the theoretical study of the hydrogen SL Ly-alpha at much higher electron densities than in the observations by Bengtson & Chester [10] and Himmel [13]. After noting that for the "unshifted" (more rigorously, central) Stark components of hydrogen SL, the quadrupole shift is to the red (which was actually well known already 6 years earlier from paper by Shoiln [21], Caby-Eyraud et al. [18] wrote: "This would explain, at least partially, the red shift observed … in the Balmer lines arising from odd upper levels" with reference to Bengtson & Chester [10]. However, first, while for the Ly-alpha line (which is the only one SL studied by Caby-Eyraud et al. [18]. the contribution of the quadrupole shift of the central Stark component to the total shift of this SL could have been significant (because for the Ly-alpha line the central component contains 2/3 of the total intensity of this line), the contribution of the quadrupole shift of the central Stark component of hydrogen SL H13, H15, H17 (studied by Bengtson & Chester [10]) to the total shift of these SL would have been miniscule (because for these SL the central component contains only between 4% and 5% of the total intensity of these lines). Second, but most importantly: for any hydrogen (or hydrogenlike) SL, after summing up the quadrupole shift over all Stark components with the allowance for the quadrupole corrections to both the energies/frequencies and the intensities, the quadrupole shift of the SL as the whole vanishes, as rigorously shown analytically byOks [17].

Therefore, the first non-vanishing contribution to the shift of the energy level is

$$s(n) = -(Z_1+Z_2)^2/(2n^2) - [-Z_1^2/(2n^2)] = -(2Z_1Z_2 + Z_2^2)/(2n^2) \quad (4)$$

Since s(n) decreases as n increases, it might seem that for the radiative transition from the upper level n to the lower level of the principal quantum number $n_0 < n$, the shift of the SL would be dominated by the shift of the lower level. However, in reality, for any level of the principal quantum number n_1 (n_1 is either n or n_0) the shift would the product of two factors: $s(n_1)$ from Equation (4) and the statistical weight $I(n_1)$ of the corresponding penetrating configuration. It will be shown below (Equation (12)), that $I(n_1)$ increases with growing n_1 much more rapidly than $\sim n_1^2$ (e.g., for relatively low density plasmas, $I(n_1)$ scales as n_1^6, so that the shift $S_{i,\,penetr}$ due to penetrating configurations scales as n_1^4).

Therefore, for high-n hydrogenic SL, for which $n >> n_0$, the shift of the lower level can be disregarded compared to the shift of the upper level. Then the contribution of penetrating configurations to the shift of hydrogenic SL can be estimated as follows:

$$S_{i,penetr} = s(n)\int_0^{u\max} dw\, P_w(w),$$
$$umax = r_{rms}(n)/R_0,\ R_0 = \left[3Z_2/(4\pi N_e)\right]^{1/3} \quad (5)$$

Here we consider the ions of charge Z_2 as the dominating ion species, while atoms/ions of the nuclear charge Z_1 are considered as a small minority (in case where Z_1 differs from Z_2). In Equation (5),

$$r_{rms}(n) = < R > = < 3n^2 - l(l+1)]/(2Z_1) >$$
$$= \left[3n^2 - n_0(n_0+2)/2\ \right]/(2Z_1) \approx 3n^2/(2Z_1) \quad (6)$$

Here <…> means the average over those sublevels of the same principal quantum number n that are involved in the radiative transition to the level $n_0 << n$, i.e., over values of l=0, 1, …, n_0 (according to the selection rules).

The distribution $P_w(w)=P_w(R/R_0)$ of the interionic distances in Equation (5) can be obtained from the binary distribution $P_u(u)=P_u(F/F_0)$ of the ion microfield (where $F=Z_2/R^2$ and $F_0=Z_2/R_0^2$, so that $u=1/w^2$) presented in papers by Held B [24,25] where these authors took into account ion-ion correlations (i.e., the ion-ion interaction) and the screening by plasma electrons– (Appendix A). Since,

$$P_w(W)\,dw = -P_u(u)\,du \quad (7)$$

Then for $P_w(w)$ we get,

$$P_w(w) = (2/w^3)P_u(1/w^2) \quad (8)$$

Using the results from papers by Held et al. [24,25] for the case of $Z_1=Z_2 \equiv Z$, the ion microfield distribution can be normalized analytically and brought to the form

$$P_u(u) = (3^{1/2}\pi/u^{5/2})exp(-1/u^{3/2} - ku^{1/2})/MeijerG$$
$$[\{\{\},\{\}\},\{\{0,\ 1/3,\ 2/3,\ 1\},\{\}\},\ k^3/27] \quad (9)$$

where Meijer G […] is the Meijer G-function and,

$$k\ = T_e Z^{3/2} v^2/(2qT_i),\ q = 15/[4(2\pi)^{1/2}] = 1.496,$$
$$v = R_0/r_{De},\ r_{De} = [T_e/(4\pi e^2 N_e)]^{1/2} \quad (10)$$

the latter being the Debye radius. A practical formula for the quantity 'v' is:

$$v\ = 8.98\mathrm{x}10^{-2}[N_e(cm^{-3})]^{1/6}/[T_e(K)]^{1/2} \quad (11)$$

n	13	14	15	16	17
Se (A)	0.0017	0.0021	0.0026	0.0032	0.0038
Si, standard (A)	0.00035	0.00055	0.00083	0.0012	0.0017

Table 2: Comparison of the electronic shift Se with the estimated standard ionic shift for hydrogen spectral lines H13 – H17.

n	Λn (A)	Se (A)	$S_{i,\,penetr}$ (A)	Stot (A)	S_{Sirius} (A)	S_{exp} (A)
13	3734	0.0017	0.032	0.034 ± 0.010	--	0.03 ± 0.03
14	3722	0.0021	0.043	0.045 ± 0.014	0.03 ± 0.05	0.00 ± 0.04
15	3712	0.0026	0.057	0.060 ± 0.018	0.09 ± 0.07	0.15 ± 0.05
16	3704	0.0032	0.073	0.076 ± 0.023	–0.007 ± 0.05	0.00 ± 0.05
17	3697	0.0038	0.093	0.10 ± 0.03	0.21 ± 0.08	0.30 ± 0.08

Table 3: Shift Si, penetrate due to penetrating ions and its sum Stot with the electronic shift Se for the hydrogen spectral lines H13 – H17, and the comparison with the shifts from paper by Bengtson and Chester [10] observed in astrophysical (S_{Sirius}) and laboratory (S_{exp}) plasmas. All shifts are in Angstrom.

Then according to Equation (8), for the distribution $P_w(w)$ entering Equation (5) we get

$$P_w(w) = 2\pi\ 3^{1/2} w^2 exp(-w^3 - k/w)/MeijerG$$
$$[\{\{\},\{\}\},\{\{0,\ 1/3,\ 2/3,\ 1\},\{\}\},\ k^3/27] \quad (12)$$

We note that the quantity k in Equation (12) scales with the electron density N_e as $N_e^{1/3}$. Therefore, for relatively low electron densities one has k << 1 and Equation (12) can be approximated as $P_w(w) = 3w^2 \exp(-w^3)$. Then the integral in Equation (5) can be calculated analytically to yield $S_{i,penetr} = s(n)\,[r_{rms}(n)/R_0]^3$. Since r_{rms} scales as n^2, then $S_{i,penetr}$ scales as n^4. As the electron density increases, the shift $S_{i,penetr}$ scales with n slower than n^4, but still very rapidly increases with growing n. The results of calculating this contribution to the shift the hydrogen SL H_{13} – H_{17} by formulas (5), (6), (12) for the parameters corresponding to the observations from paper by Bengtson and Chester [10] ($N_e = 1.2 \times 10^{13}$ cm^{-3}, $Z_1 = Z_2 = 1$), are shown in Table 2 in the column $S_{i,penetr}$. The sum $S_{i,penetr} + S_e$ is shown in the column Stot. The theoretical error margin is shown only for the latter and it is primarily due to the approximate way of estimating $S_{i,penetr}$.

The following can be seen from Table 3:

1. For the SL H_{13}, there is an excellent agreement between the total theoretical shift Stot and the experimental shift S_{exp}. No data for the shift of this SL from Sirius.

2. For the SL H_{14}, there is a good agreement of the total theoretical shift with the shift of this SL observed from Sirius and a satisfactory agreement (within the error margins) with the experimental shift of this SL.

3. For the SL H_{15}, there is a good agreement of the total theoretical shift with the shift of this SL observed from Sirius and a satisfactory agreement (almost within the error margins) with the experimental shift of this SL.

4. For the SL H_{16}, there is a satisfactory agreement (within the error margins) of the total theoretical shift with both the shift of this SL observed from Sirius and the experimental shift of this SL.

5. For the SL H_{17}, there is a satisfactory agreement (within the error margins) of the total theoretical shift with the shift of this SL observed from Sirius, but a disagreement with the experimental shift of this

SL; however, the latter disagreement is not anymore by two orders of magnitude, as it was the case before the present paper, but rather just by a factor of two (after allowing for the error margins).

Justification of the quasistatic description of the penetrating configurations in hydrogen plasmas can be found in Appendix B.

Conclusion

The present paper was motivated by the fact that high-n hydrogen SL (n=13–17), studied in in the astrophysical and laboratory observations at Ne ~ 10^{13} cm^{-3} by Bengtson and Chester [10], exhibited red shifts by orders of magnitude greater than the theoretical shifts known up to now. We introduced an additional source of the shift of high-n hydrogenic SL arising from the configurations where the nearest perturbing ion is within the radiating atom/ion ("penetrating configurations"). We demonstrated that for high-n hydrogen SL it makes the primary contribution to the total red shift. We showed that for the conditions of the astrophysical and laboratory observations from paper by Bengtson and Chester [10], this additional red shift is by orders of magnitude greater than the theoretical shifts known up to now. The comparison with the red shifts observed in paper by Bengtson and Chester [10] demonstrated that the allowance for this additional red shift removes the existed huge discrepancy–the discrepancy by orders of magnitude–between the observed and theoretical shifts.

We emphasize that the primary focus of the present paper was to bring to the attention of the research community a new source of shifts of hydrogenic lines and to show that it is the dominant source of shifts of spectral lines corresponding to the radiative transitions from a level n to a level $n_0 << n$. This is an important fundamental result in its own right. As for the application of this fundamental result to the laboratory and astrophysical observations by Bengtson and Chester [10], we note the following. While the allowance for this shift brought the theory by orders of magnitude closer to the observations by Bengtson and Chester [10], it cannot be interpreted as the ultimate explanation of the observations by Bengtson and Chester [10] (e.g., for lines H_{14} and H_{16}, while there is an agreement within the combined error margins, there is still no explanation why the most probable value of the observed shift for these two lines was zero).

Another potential application of this new source of shifts might have been to Radio Recombination Lines (RRL), i.e. to hydrogen lines corresponding to radiative transitions from a level n >>1 to one of the neighboring levels n_0=n–p, where p << 1. However, it turns out that for RRL, this shift is about 5 orders of magnitude smaller than the width, thus making practically impossible to detect such shift (Appendix C). There are two reasons for this result. First, this shift is proportional to the electron density N_e and for H II regions emitting RRL, N_e is by 9 or 10 orders of magnitude smaller than for laboratory and astrophysical plasmas studied by Bengtson and Chester [10]. Second, for RRL one has n and n_0 very close to each other (both being in the range between 100 and about 200). In this situation, the contribution from level n to the shift (which would lead to the red shift of a particular PRL) and the contribution from level n_0 to the shift (which would lead to the blue shift of the same PRL) almost cancel each other.

More rigorously, the resulting shift of RRL increases with growing n much slower than for radiative transitions from level n to level n_0 << n (Appendix C). Therefore, the fact that for RRL the values of n are by about one order of magnitude greater than for observations by Bengtson and Chester [10] cannot override the decrease of the electron density by 9 or 10 orders of magnitude.

Finally we emphasize that in the present paper we calculated this new red shift approximately–just the get the message across. We hope that our results would motivate further observational and theoretical studies of the shifts of high-n hydrogenic spectral lines in astrophysical and laboratory plasmas.

Appendix A: Details on the Ion Micro-Field Distribution

Held et al. [24] derived the ion microfield distribution at a charged point ($P_u(u)$ in our notation, u=F/F_0), as well as the related distribution of interionic distances ($P_w(w)$ in our notation, w=R/R_0), taking into account ion-ion correlations (i.e., ion-ion interaction) and the screening by plasma electrons. For relatively small interionic distances, relevant to our study of the shift by penetrating ions, the unnormalized distribution given by Equation (67) from Held et al. [24] can be represented in our notations as follows:

$$P_w\left(w\right) \sim (qN_i / N_e)g\left(w\right)w^2 exp[-\int_0^w dw' w'^2 (qN_i / N_e)g\left(w'\right)] \quad \text{(A.1)}$$

where the factor g(w) incorporates ion-ion correlations and the screening by plasma electrons. If one would disregard ion-ion correlations and the screening by plasma electrons, so that it would be g(w)=1, then the normalized distribution would simplify to:

$$P_w\left(w\right) = 3w^2 exp(-w^3) \quad \text{(A.2)}$$

The allowance for ion-ion correlations and the screening by plasma electrons adds additional exponential factor, which in our notation is exp(– k/w) where k is given in Equation (10). As a result, the normalized distribution P_w(w) takes the form given by Equation (12).

Appendix B: Justification of the Quasistatic Description of the Penetrating Configurations in Hydrogen Plasmas

From the theory of the Stark broadening of hydrogen lines in plasmas it is well-known that the quasistatic description of the interaction of the perturbing ion with the radiating hydrogen atom is valid as long as the internuclear separation is much smaller than the ion Weisskopf radius ρ_{Wi} (see, e.g., review by Lisitsa [26]), where,

$$\rho wi = (n^2\hbar / m_e) < 1/Vi > = (n^2\hbar / m_e)\ [2M_{reduced} / \left(\pi T\right)]^{1/2} \quad \text{(B.1)}$$

Here <1/V_i> is the inverse ion velocity averaged over the Maxwell distribution, $M_{reduced}$ is the reduced mass of the pair perturber-radiator. (In this Appendix we do not use the atomic units.) For hydrogen plasmas, $M_{reduced}$=M_p/2, where M_p is the proton mass, so that

$$\rho wi = (n^2\hbar / m_e)\ [2M_p / \left(\pi T\right)]^{1/2} \quad \text{(B.2)}$$

The largest internuclear separation, involved in calculating the shift of hydrogen lines due to penetrating configurations, is

$$r_{rms} = 3n^2 a_0 / 2 \quad \text{(B.3)}$$

where a_0 is the Bohr radius (according to Equation (6) with Z_1=1). Therefore, for the ratio r_{rms}/ρ_{Wi} we obtain:

$$\begin{aligned} r_{rms} / \rho wi &= \left(3\pi^{1/2}/2\right)\left(\hbar c / e^2\right)\left[T / \left(M_p c^2\right)\right]^{1/2} \\ &= \left(3\pi^{1/2}/2\right)137 \\ &\left[T\left(eV\right) / \left(9.38\text{x}10^8\right)\right]^{1/2} = \left[T\left(eV\right) / \left(7.1\text{x}10^3\right)\right]^{1/2} \end{aligned} \quad \text{(B.4)}$$

Thus, the quasistatic description of penetrating configurations in hydrogen plasmas is valid as long as the temperature is:

$$T << 7.1\ \text{KeV} = 8.2\text{x}10^7 K \quad \text{(B.5)}$$

Obviously this condition is fulfilled in the laboratory and astrophysical plasmas studied by Bengtson and Chester [10], as well as in many other laboratory and astrophysical plasmas.

Appendix C: No Measurable Shifts of Radio Recombination Lines

In the well-known paper by Bell et al. [27], the authors measured widths of Radio Recombination Lines (RRL) from several H II regions, including Orion A. Their primary finding was that the width of RRL of the principal quantum number n up 180 increased with the growing n, but for RRL of n > 180 the widths decreased with the growing n. Recently Alexander and Gulyaev [28] presented the newest observations of RRL from Orion nebula. They also found that the width of RRL of the principal quantum number n up 180 increased with the growing n.

As for the RRL of n ~ 200 and higher observed by Bell et al., [27] and Alexander and Gulyaev [28] point out the following. Bell et al. [27] applied the frequency switching method to the same spectrum six times successively, which made their method increasingly insensitive to line broadening as the line width increased and exceeded the frequency switching offset parameter.

Alexander and Gulyaev [28] demonstrated that the narrowing of RRL reported by Bell et al. [27] is apparent: their method effectively filtered out Stark broadening for n ~ 200 and higher. For this range of n, most of the width measurements by Bell et al. [27] were below the Doppler width and increasingly below 3σ in signal-to-noise ratio, which is a manifestation of limitations in the use of the frequency switching method multiple times in succession.

Therefore, here we estimate the shift by penetrating ions for RRL up to n=180 and compare it with the measured width. For the extremely low electron densities characteristic for H II regions ($N_e \sim 4000$ cm^{-3} or less according to Bell et al. [27], $N_e \sim 5000$ cm^{-3} according to Alexander and Gulyaev [28], the distribution P(w) of the relative separation $w=R/R_0$, given by Equation (12), can be simplified, so that after the integration in Equation (5) the result for the shift by penetration ions simplifies to (for $Z_1=Z_2=1$):

$$S_{i,penetr} = -81(n^4 - n_0^4)/[16\,R_0^3] \tag{C.2}$$

The relative shift $\delta S_{i,\,penetr}$, defined as ratio of this shift to the unperturbed frequency of the particular RRL is:

$$\delta S_{i,penetr} = -81 n^2 n_0^2 (n^2 + n_0^2)/[8\,R_0^3] \tag{C.3}$$

Since RRL are characterized by $n_0=n-p$, where p << n, then Equation (C.2) can be simplified to:

$$\delta S_{i,penetr} = -81 n^6 / \left[4\,R_0^3\right] \tag{C.3}$$

After substituting $1/R_0^3=4\pi N_e/3$ and returning from the atomic units of N_e to the CGS units, we obtain:

$$\begin{aligned}\delta S_{i,penetr} &= -27\pi\, n^6 N_e a_0^3 \\ &= -1.26\text{x}10^{-23} n^6 N_e \left[cm^{-3}\right]\end{aligned} \tag{C.4}$$

(a_0 is the Bohr radius).

For n=180 and N_e = (4000–5000) cm^{-3}, Equation (C.4) yields $\delta S_{i,\,penetr}$ = (1-2) × 10^{-6}. The relative width δW (i.e., the ratio of the width to the unperturbed frequency of the RRL), as measured by Bell et al. and Alexander J, Gulyaev S [27] was δW ~ 0.1 for n ~ 180. In other words, the measured width exceeds the shift (caused by penetrating ions) by 5 orders of magnitude, so that it was impossible to detect it.

To conclude this Appendix, let us briefly discuss the experimental results by LaSalle, Nee and Griem [29]. These authors presented profiles of hydrogen lines measured in a laboratory plasma–the lines corresponding to the radiative transitions between level n and n-1 (so called n-alpha lines) for n=12, 13 and 14. While their focus was on the experimental width of these lines, they also mentioned some experimental red shift, such as, e.g., (0.2 ± 0.2) μm for Ne between 3.4 × 10^{14} cm^{-3} and 5.8 × 10^{14} cm^{-3}. For example for the line originating from n=12, it corresponds to the relative shift δS_{exper} = (0.003 ± 0.003). If one would formally apply Equation (C.4) to this case, one would get the theoretical relative shift $\delta S_{i,\,penetr}$ at least two times higher.

However, in the experiment by LaSalle, Nee and Griem [29], the electron density N_e was by 11 orders of magnitude higher than in observations by Bell et al. [27] and by Alexander and Gulyaev [28] (and by 30-50 times higher than in the experiment by Bengtson and Chester [10]). Therefore, the low density approximation of the distribution P(w) of the relative separation $w=R/R_0$, employed in the derivation of Equation (B.4), is not justified. The more accurate calculation, based on Equations (5) and (12), brings $\delta S_{i,\,penetr}$ to practically an agreement with δS_{exper} = (0.003 ± 0.003) within the combined error margins of $\delta S_{i,\,penetr}$ and δS_{exper}.

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