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Stark Broadening of Hydrogenlike Spectral Lines by Plasma Electrons: The Allowance for Non-Hyperbolic Trajectories

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ABSTRACT: The broadening of hydrogenlike spectral lines in plasmas by electrons is treated in the so-called Conventional Theory (CT) under the assumption that the perturbing electrons move along hyperbolic trajectories in the Coulomb field of the effective charge $Z - 1$ (in atomic units), where Z is the nuclear charge of the radiating ion. Thus, the CT assumed that the motion of the perturbing electron can be described in frames of a two-body problem, one particle being the perturbing electron and the other "particle" being the charge $Z - 1$. However, in reality it is a three-body problem, involving the perturbing electron, the nucleus, and the bound electron, so that trajectories of the perturbing electrons should be more complicated. In the present paper we take this into account via the standard analytical method of separating rapid and slow subsystems by using the fact that the characteristic frequency of the motion of the bound electron around the nucleus is much higher than the characteristic frequency of the motion of the perturbing electron around the radiating ion.

By applying this method we obtain more accurate analytical results for the electron broadening operator than in the CT. We show by examples of the electron broadening of the Lyman lines of He II that the allowance for this effect increases with the electron density N_e, becomes significant already at $N_e \sim 10^{17}$ cm^{-3} and very significant at higher densities. We also briefly discuss a paper by Baryshnikov and Lisitsa (Sov. Phys. JETP **53** (1981) 471) where the fundamental symmetry of the effective potential for this problem was used in a different way.

Key words: Stark broadening, hydrogenlike spectral lines, non-hyperbolic trajectories, analytical results

1. INTRODUCTION

In the so-called Conventional Theory (CT) of the Stark broadening of hydrogenlike spectral lines by plasma electrons, developed by Griem and Shen [1] and later presented also in books [2, 3], the perturbing electrons are considered moving along hyperbolic trajectories in the Coulomb field of the effective charge Z – 1 (in atomic units), where Z is the nuclear charge of the radiating ion. (The CT is sometimes called also the standard theory; further advances in the theory of the Stark broadening of hydrogenlike spectral lines by plasma electrons can be found, e.g., in books [4, 5] and references therein.) In other words, in the CT there was made a simplifying assumption that the motion of the perturbing electron can be described in frames of a two-body problem, one particle being the perturbing electron and the other "particle" being the charge Z – 1.

However, in reality one have to deal with a three-body problem: the perturbing electron, the nucleus, and the bound electron. Therefore, trajectories of the perturbing electrons should be more complicated.

In the present paper we take this into account by using the standard analytical method of separating rapid and slow subsystems – see, e.g., book [6]. The characteristic frequency of the motion of the bound electron around the nucleus is much higher than the characteristic frequency of the motion of the perturbing electron around the radiating ion. Therefore the former represents the rapid subsystem and the latter represents the slow subsystem. This approximate analytical method allows a sufficiently accurate treatment in situations where the perturbation theory fails – see, e.g., book [6].

By applying this method we obtain more accurate analytical results for the electron broadening operator than in the CT. We show by examples of the electron broadening of the Lyman lines of He II that the allowance for this effect increases with the electron density N_e, becomes significant already at $N_e \sim 10^{17}$ cm^{-3} and very significant at higher densities.

2. ANALYTICAL RESULTS

In the CT the electron broadening operator is expressed in the form (see, e.g., paper [1])

$$\Phi_{ab} \equiv 2\pi v\, Ne \int d\rho\, \rho \{S_a S_b^* - 1\}, \tag{1}$$

where N_e, v, and ρ are the electron density, velocity, and impact parameter, respectively; $S_a(0)$ and $S_b(0)$ are the S matrices for the upper (a) and lower (b) states involved in the radiative transition, respectively; {…} stands for the averaging over angular variables of vectors **v** and **ρ**. Further in the CT, the collisions are subdivided into weak and strong. The weak collisions are treated by the time-dependent perturbation theory. The impact parameter, at which the formally calculated expression $\{S_a S_b^* - 1\}$ for a weak collision starts violating the unitarity of the S-matrices, serves as the boundary between the weak and strong collisions and is called Weisskopf radius ρ_{We}.

So, in the CT the integral over the impact parameter diverges at small ρ. Therefore in the CT this integral is broken down in two parts: from 0 to ρ_{We} (strong collisions) and from ρ_{We} to ρ_{max} for weak collisions. The upper cutoff ρ_{max} (typically chosen to be the Debye radius $\rho_D = [T/(4\pi e^2 N_e)]^{1/2}$, where T is the electron temperature) is necessary because this integral diverges also at large ρ.

In the CT, after calculating the S matrices for weak collisions, the electron broadening operator becomes (*in atomic units*)

$$\Phi_{ab}^{weak} \equiv C \int_{\rho_{we}}^{\rho_{max}} d\rho\, \rho \sin^2 \frac{\Theta(\rho)}{2} = \frac{C}{2} \int_{\Theta_{min}}^{\Theta_{max}} d\Theta \frac{d\rho^2}{d\Theta} \sin^2 \frac{\Theta}{2}, \tag{2}$$

where Θ is the scattering angle for the collision between the perturbing electron and the radiating ion (the dependence between Θ and ρ being discussed below) and the plasma electron and the operator C is

$$C = -\frac{4\pi}{3} N_e \left[\int_0^\infty dv\, v^3 f(v) \right] \frac{m^2}{(Z-1)^2} (r_a - r_b^*)^2. \tag{3}$$

Here $f(v)$ is the velocity distribution of the perturbing electrons, $\boldsymbol{r}$ is the radius-vector operator of the bound electron (which scales with Z as $1/Z$), and m is the reduced mass of the system "perturbing electron – radiating ion".

In the *CT* the scattering occurs in the effective Coulomb potential, so that the trajectory of the perturbing electron is hyperbolic and the relation between the impact parameter and the scattering angle is given by

$$\rho^{(0)} = \frac{Z-1}{mv^2} \cot \frac{\Theta}{2}. \tag{4}$$

In the present paper we consider the realistic situation where trajectories of the perturbing electrons are more complicated because the perturbing electron, the nucleus, and the bound electron should be more accurately treated as the three-body problem. We use the standard analytical method of separating rapid and slow subsystems – see, e.g., book [6]. It is applicable here because the characteristic frequency v_{Te}/ρ_{We} of the variation the electric field of the perturbing electrons at the location of the radiating ion is much smaller than the frequency Ω_{ab} of the spectral line (the latter, e.g., in case of the radiative transition between the Rydberg states would be the Keppler frequency or its harmonics) – more details are presented in Appendix.

The first step in this method is to "freeze" the slow subsystem (perturbing electron) and to find the analytical solution for the energy of the rapid subsystem (the radiating ion) that would depend on the frozen coordinates of the slow subsystem (in our case it will be the dependence on the distance *R* of the perturbing electron from the radiating ion). To the first non-vanishing order of the *R*-dependence, the corresponding energy in the parabolic quantization is given by

$$E_{nq}(R) = \frac{Z^2}{n^2} + \frac{3\,n\,q}{2\,Z\,R^2}, \tag{5}$$

where n and $q = n_1 - n_2$ are the principal and electric quantum numbers, respectively; n_1 and n_2 are the parabolic quantum numbers.

The next step in this method is to consider the motion of the slow subsystem (perturbing electron) in the "effective potential" V_{eff}(R) consisting of the actual potential plus E_{nq}(R). Since the constant term in Eq. (5) does not affect the motion, the effective potential for the motion of the perturbing electron can be represented in the form

$$V_{eff}(R) = -\frac{\alpha}{R} + \frac{\beta}{R^2}, \qquad \alpha = Z - 1. \tag{6}$$

For the spectral lines of the Lyman series, since the lower (ground) state *b* of the radiating ion remains unperturbed (up to/including the order $\sim 1/R^2$), the coefficient β is

$$\beta = \frac{3 n_a q_a}{2\,Z}. \tag{7}$$

For other hydrogenic spectral lines, for taking into account both the upper and lower states of the radiating ion, the coefficient β can be expressed as

$$\beta = \frac{3(n_a q_a - n_b q_b)}{2\,Z} \tag{8}$$

The motion in the potential from Eq. (6) allows an exact analytical solution. In particular, the relation between the scattering angle and the impact parameter is no longer given by Eq. (4), but rather becomes (see, e.g., book [7])

$$\Theta = \pi - \frac{2}{\sqrt{1 + \frac{2m\beta}{M^2}}} \arctan \sqrt{\frac{4E}{\alpha^2}\left(\beta + \frac{M^2}{2m}\right)}. \tag{9}$$

Here *E* and *M* are the energy and the angular momentum of the perturbing electron, respectively. We can rewrite the angular momentum in terms of the impact parameter ρ as

$$M = m\,v\,\rho \tag{10}$$

Then a slight rearrangement of Eq. (9) yields

$$\tan\left(\frac{n - \Theta}{2}\sqrt{1 + \frac{2\beta}{m v^2 \rho^2}}\right) = \frac{v}{\alpha}\sqrt{m^2 v^2 \rho^2 + 2m\beta}. \tag{11}$$

After solving Eq. (11) for ρ and substituting the outcome in Eq. (2), a more accurate expression for the electron broadening operator can be obtained. However, Eq. (11) does not have an exact analytic solution for ρ so that this could be done only numerically.

In the present paper, to get the message across in the simplest form, we will provide an approximate analytical solution of Eq. (11) by expanding it in powers of β. This yields (keeping up to the first power of β)

$$\tan\left(\frac{\pi-\Theta}{2}\right)+\left(\frac{\pi-\Theta}{2}\right)\left[1+\tan^2\left(\frac{\pi-\Theta}{2}\right)\right]\frac{\beta}{m\,v^2\rho^2}\approx\frac{m\,v^2\rho}{\alpha}+\frac{\beta}{\alpha\rho}. \tag{12}$$

We seek the analytical solution for ρ in the form $\rho \approx \rho^{(0)} + \rho^{(1)}$, where $\rho^{(0)}$ corresponds to $\beta = 0$ (and was given by Eq. (4)) and $\rho^{(1)} << \rho^{(0)}$. Substitution of $\rho \approx \rho^{(0)} + \rho^{(1)}$ into Eq. (12) yields the expression

$$\frac{(\pi-\Theta)\beta}{2mv^2\rho^{(0)^2}\sin^2\frac{\Theta}{2}}-\frac{\beta}{\alpha\,\rho^{(0)}}\approx\frac{m\,v^2\rho^{(1)}}{\alpha}. \tag{13}$$

After solving Eq. (13) for $\rho^{(1)}$, we get the expression for ρ:

$$\rho\approx\frac{\alpha}{m\,v^2}\cot\frac{\Theta}{2}+\frac{\beta}{\alpha}\left(\frac{\pi-\Theta}{2\cos^2\frac{\Theta}{2}}-\tan\frac{\Theta}{2}\right). \tag{14}$$

As a reminder, our goal is to perform the integration in Eq. (1) for obtaining a more accurate analytical result for the electron broadening operator. This can be more easily accomplished by performing the integration over Θ instead of ρ. For this purpose, first we square Eq. (14)

$$\rho^2\approx\frac{\alpha^2}{m^2v^4}\cot^2\frac{\Theta}{2}+\frac{\beta}{m\,v^2}\left(\frac{\pi-\Theta}{\sin\frac{\Theta}{2}\cos\frac{\Theta}{2}}-1\right), \tag{15}$$

where only the first order terms in β have been kept for consistency. To make formulas simpler, we denote $\phi = \Theta/2$. After differentiating Eq. (15) with respect to ϕ, we obtain

$$\frac{d\rho^2}{d\phi}\approx-\frac{\alpha^2}{m^2v^4}\frac{2\cot\phi}{\sin^2\phi}-\frac{2\beta}{mv^2}\left[\left(\frac{1}{\sin\phi\cos\phi}\right)+\left(\frac{\pi}{2}-\phi\right)\left(\frac{1}{\sin^2\phi}-\frac{1}{\cos^2\phi}\right)\right] \tag{16}$$

After substituting in the utmost right side of Eq. (2) first $\Theta = 2\phi$ and then $\frac{d\rho^2}{d\phi}$ from Eq. (16), the contribution of the weak collisions to the electron broadening operator becomes

$$\Phi_{ab}^{\ weak}=-C\left[\frac{\alpha^2}{m^2v^4}\int_{\phi_{\min}}^{\phi_{\max}}\cot\phi\,d\phi+\frac{\beta}{m\,v^2}\int_0^{\frac{\pi}{2}}\tan\phi\,d\phi+\frac{\beta}{mv^2}\int_0^{\frac{\pi}{2}}\left(\frac{\pi}{2}-\phi\right)(1-\tan^2\phi)d\phi\right]. \tag{17}$$

In Eq. (17), in the two correction terms proportional to β, we extended the integration over the full range of the variation of the angle ϕ. The corresponding minor inaccuracy would not contribute significantly to the electron broadening operator, since the terms involving β are considered to be a relatively small correction to the first term in Eq. (17).

Performing the integrations in Eq. (17) we obtain:

$$\Phi_{ab}^{weak} = -\frac{4\pi}{3} N_e (r_a - r_b^*)^2 \left[\int_0^\infty dv \frac{f(v)}{v}\right]\left[\log\frac{\sin\phi_{\max}}{\sin\phi_{\min}} + \frac{mv^2\beta}{(Z-1)^2}\left(\frac{\pi^2}{4}-1\right)\right]. \tag{18}$$

Now we add the CT estimate for the contribution of strong collisions

$$\Phi_{ab}^{strong} \approx \pi v N_e \, \rho_{We}^{\ 2}, \tag{19}$$

where ρ_{We} corresponds to ϕ_{max}. Expressions for ϕ_{max} and ϕ_{min} are given in paper [1] (in Eqs. (9) and (10a)) as follows

$$\sin\phi_{\max} = \sqrt{\frac{3}{2}} \frac{Z(Z-1)}{(n_a^2 - n_b^2) m v}, \tag{20}$$

$$\sin\phi_{\min} = \frac{\dfrac{Z-1}{m v^2 \rho_D}}{\sqrt{1 + \dfrac{(Z-1)^2}{m^2 v^4 \rho_D^2}}} \tag{21}$$

It should be emphasized that the factor $\left(n_a^2 - n_b^2\right)$ in the denominator of the right side of Eq. (20) was an approximate allowance by the authors of paper [1] for the contribution of the lower level b while estimating the operator $(\boldsymbol{r}_a - \boldsymbol{r}_b^*)$ for hydrogenic lines of spectral series other than the Lyman lines. However, for the Lyman lines the lower (ground) level does not contribute to electron broadening operator, so that for the Lyman lines Eq. (20) should be simplified as follows:

$$\sin\phi_{\max} = \sqrt{\frac{3}{2}} \frac{Z(Z-1)}{n_a^2 m v} \tag{22}$$

We also note that at relatively small velocities of perturbing electrons, the right side of Eq.(20) or Eq. (22) could exceed unity. In this case one should set $\sin\phi_{max} = 1$, what corresponds to $\rho_{\min} = 0$, so that there would be no contribution from strong collisions. Typically, the range of such small velocities has a very low statistical weight in the electron velocity distribution.

After substituting the above formulas for $\sin\phi_{max}$ and $\sin\phi_{min}$ into Eq. (17), and combining the contributions from weak and strong collisions, we obtain the final results for the electron broadening operator:

$$\Phi_{ab}(\beta) = -\frac{4\pi}{3} N_e (r_a - r_b^*)^2 \left[\int_0^\infty dv \frac{f(v)}{v}\right]\left\{\frac{1}{2}\left[1 - \frac{3}{2}\frac{Z^2(Z-1)^2}{(n_a^2-n_b^2)^2 m^2 v^2}\right] + \log\left[\sqrt{\frac{3}{2}} \frac{Z v \rho_D}{(n_a^2-n_b^2)} \sqrt{1+\left(\frac{Z-1}{m v^2 \rho_D}\right)^2}\right] + \frac{mv^2\beta}{(Z-1)^2}\left(\frac{\pi^2}{4}-1\right)\right\} \tag{23}$$

for the non-Lyman lines and

$$\Phi_{ab}(\beta) = -\frac{4\pi}{3} N_e (r_a - r_b^*)^2 \left[\int_0^\infty dv \frac{f(v)}{v}\right] \left\{ \frac{1}{2}\left[1 - \frac{3}{2}\frac{Z^2 (Z-1)^2}{n_a^4 m^2 v^2}\right] + \log\left[\sqrt{\frac{3}{2}}\frac{Z v \rho_D}{n_a^2}\sqrt{1+\left(\frac{Z-1}{m v^2 \rho_D}\right)^2}\right] + \frac{m v^2 \beta}{(Z-1)^2}\left(\frac{\pi^2}{4} - 1\right)\right\} \quad (24)$$

for the Lyman lines. Here and below log [...] stands for the natural logarithm.

3. SIGNIFICANCES OF THE EFFECT

In order to determine the significance of this effect, it is necessary then to evaluate the ratio

$$ratio = \frac{\frac{3}{2}\frac{m v^2 (n_a q_a - n_b q_b)}{(Z-1)^2}\left(\frac{\pi^2}{4} - 1\right)}{\frac{1}{2}\left[1 - \frac{3}{2}\frac{Z^2 (Z-1)^2}{(n_a^2 - n_b^2)^2 m^2 v^2}\right] + \log\left[\sqrt{\frac{3}{2}}\frac{Z v \rho_D}{(n_a^2 - n_b^2)}\sqrt{1+\left(\frac{Z-1}{m v^2 \rho_D}\right)^2}\right]} \quad (25)$$

for the non-Lyman lines or the ratio

$$ratio = \frac{\frac{3}{2}\frac{m v^2 n_a q_a}{(Z-1)^2}\left(\frac{\pi^2}{4} - 1\right)}{\frac{1}{2}\left[1 - \frac{3}{2}\frac{Z^2 (Z-1)^2}{n_a^4 m^2 v^2}\right] + \log\left[\sqrt{\frac{3}{2}}\frac{Z v \rho_D}{n_a^2}\sqrt{1+\left(\frac{Z-1}{m v^2 \rho_D}\right)^2}\right]} \quad (26)$$

for the Lyman lines.

Below we present numerical examples for several Lyman lines. As it is customary in the Stark broadening theory, instead of the integration over velocities, for the numerical examples we use the mean thermal velocity v_T of the perturbing electrons. In atomic units, the mean thermal velocity v_T, the Debye radius ρ_D, and the reduced mass can be expressed as follows.

$$v_T = 0.1917\sqrt{\frac{T(eV)}{m}} \quad \rho_D = 1.404 \times 10^{11}\sqrt{\frac{T(eV)}{N_e(cm^{-3})}} \quad m = \frac{1 + \frac{m_e}{A m_p}}{1 + \frac{2 m_e}{A m_p}}, \quad (27)$$

where m_e is the electron mass, m_p is the proton mass, and A is the atomic number of the radiating ion ($A \approx 2Z$).

Table 1 presents the values of the ratio from Eq. (26) for several Lyman lines of He II at the temperature T = 8 eV and the electron density $N_e = 2x10^{17}$ cm^{-3}.

Table 1
Ratio from Eq. (26) for the Stark components of several Lyman lines of He II at the temperature $T = 8\ eV$ and the electron density $N_e = 2 \times 10^{17}\ cm^{-3}$

N	|*q*|	*ratio*
2	1	0.3261
3	1	0.3748
3	2	0.7496
4	1	0.5156
4	2	1.0311
4	3	1.5467

Figure 1 shows the ratio from Eq. (26) versus the electron density N_e for the Stark components of the electric quantum number $|q| = 1$ of Lyman-alpha ($n = 2$), Lyman-beta ($n = 3$), and Lyman-gamma ($n = 4$) lines of He II at the temperature $T = 8\ eV$.

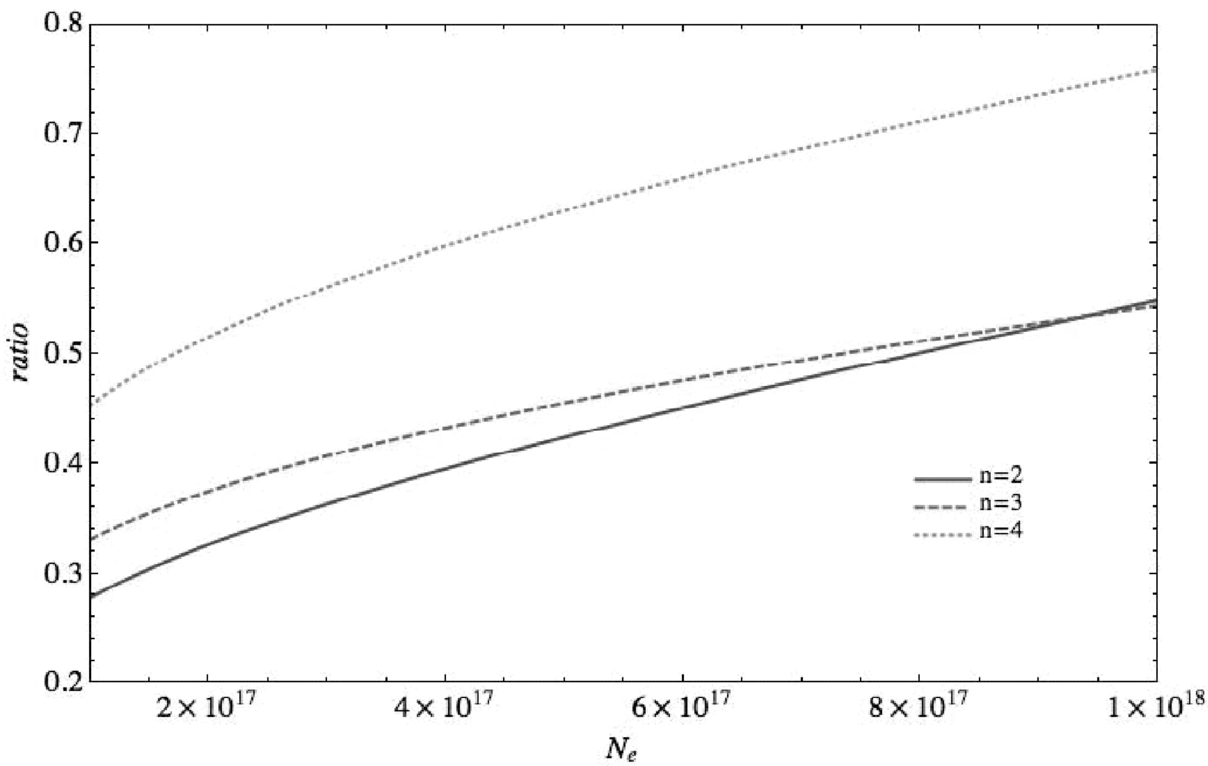

Figure 1: Ratio from Eq. (26) versus the electron density N_e for the Stark components of the electric quantum number $|q| = 1$ of Lyman-alpha ($n = 2$), Lyman-beta ($n = 3$), and Lyman-gamma ($n = 4$) lines of He II at the temperature $T = 8\ eV$

It is seen that for the electron broadening of the Lyman lines of He II, the allowance for the effect under consideration is indeed becomes significant already at electron densities $N_e \sim 10^{17}\ cm^{-3}$ and increases with the growth of the electron density. It should be noted that when the ratio, formally calculated by Eq. (26), becomes comparable to unity, this is the indication that the approximate analytical treatment based on expanding Eq. (11) up to the first order of parameter β, is no longer valid. In this case the calculations should be based on solving Eq. (11) with respect to ρ without such approximation.

4. CONCLUSIONS

In this paper we considered the electron broadening of hydrogenlike spectral lines in plasmas more accurately than in the CT. In distinction to the CT, we treated it as a three-body problem involving the perturbing electron, the nucleus, and the bound electron. We employed the standard analytical method of separating rapid and slow subsystems by using the fact that the characteristic frequency of the motion of the bound electron around the nucleus is much higher than the characteristic frequency of the motion of the perturbing electron around the radiating ion.

With the help of this method we obtained more accurate analytical results for the electron broadening operator compared to the CT. By examples of the electron broadening of the Lyman lines of He II, we demonstrated that the allowance for this effect becomes significant at electron densities $N_e \sim 10^{17}$ cm^{-3} and very significant at higher densities.

We mention that in 1981, Baryshnikov and Lisitsa [8] published very interesting results for the electron broadening of hydrogenlike spectral lines in plasmas (also presented later in book [9]) in frames of the quantum theory of the dynamical Stark broadening, while we obtained our results in frames of the semiclassical theory of the dynamical Stark broadening, just as in the CT. (For clarity: in the semiclassical theory, the radiating atom/ion is treated quantally, while perturbing electrons classically; in the quantum theory both the radiating atom/ion and perturbing electrons are treated quantally.) Both in paper [8] and in our paper, there was used the underlying symmetry of the class of potentials $V(R) = -A/R + B/R^2$ for obtaining analytical solutions.

A specific result for the line width Baryshnikov and Lisitsa [8] obtained for Lyman lines in the classical limit using the impact approximation, as presented in their Eqs. (4.5) and (4.6). We compared their results from Eqs. (4.5) and (4.60) with the CT [1] for He II Lyman lines. It turned out that for $N_e \sim (10^{17} - 10^{18})$ cm^{-3}, i.e. for the range of electron densities, in which the overwhelming majority of measurements of the width of He II lines were performed, Baryshnikov-Lisitsa's line width exceeds the CT line width by two orders of magnitude or more. In view of the fact that the width of He II lines, measured by various authors in benchmark experiments (i.e., experiments where plasma parameters were measured independently of the line widths), never exceeded the CT width by more than a factor of two (see, e.g., benchmark experiments [10-12]), this seems to indicate that something might be incorrect in Eqs. (4.5) and (4.6) from paper [8] (though methodologically it was a very interesting paper). In distinction, the corrections to the CT that we introduced in the present paper, do not exceed the factor of two for He II lines in the range of $N_e \sim (10^{17} - 10^{18})$ cm^{-3}.

Appendix A. Validity of using the analytical method based on separating rapid and slow subsystems

The characteristic frequency of the motion of the perturbing electron around the radiating ion in the process of the Stark broadening of spectral lines is the so-called Weisskopf frequency

$$\omega_{We} = \frac{v_T}{\rho_{We}} \sim \frac{Z m v_T^2}{(n_a^2 - n_b^2)\hbar} \sim \frac{ZT}{(n_a^2 - n_b^2)\hbar}. \tag{A.1}$$

The characteristic frequency of the motion of the bound electron around the nucleus is the frequency of the spectral line

$$\Omega = \frac{Z^2 U_H}{\hbar}\left(\frac{1}{n_b^2} - \frac{1}{n_a^2}\right), \tag{A.2}$$

where U_H is the ionization potential of hydrogen. The ratio of these two frequencies is

$$\frac{\omega_{We}}{\Omega} \sim \left(\frac{T}{ZU_H}\right)\left[\frac{n_a^2 n_b^2}{(n_a^2 - n_b^2)^2}\right]. \tag{A.3}$$

For the simplicity of estimating this ratio, let us consider $n_a >> n_b$, so that

$$\frac{\omega_{We}}{\Omega} \sim \left(\frac{T}{Z\ n_a^2 U_H} \right) << 1 \qquad \text{(A.4)}$$

as long as

$$T(eV) << (13.6\,eV)\,Z\,n_a^2. \qquad \text{(A.5)}$$

For example, for $Z = 2$ the above validity condition becomes

$$T(eV) << (27.2\,eV)\ n_a^2. \qquad \text{(A.6)}$$

and is satisfied for a broad range of temperatures, at which He II spectral lines are observed in plasmas.

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