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Allowance for the Scattering on the Atomic Electric Dipole in the Stark Broadening of Hydrogen Spectral Lines in Plasmas

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ABSTRACT: The Stark broadening (SB) of hydrogen lines (H-lines, including deuterium and tritium lines) is an important diagnostic tool for many applications. Examples are (but not limited to) magnetically-controlled fusion, low-temperature technological discharges for plasma processing, laser-induced breakdown spectroscopy, and astrophysics. The most "user-friendly" are semiclassical theories of the SB of H-lines – because their results can be expressed analytically in a relatively simple form for any H-line. Within the semiclassical theories, the simplest is the so-called Conventional Theory (CT), which is frequently referred to as Griem's theory – as presented in Kepple-Griem paper (Phys. Rev. **173** (1968) 317) and in Griem's book ("Spectral Line Broadening by Plasmas", Academic, New York, 1974). While by now there are several significantly more advanced semiclassical "non-CT" theories of the SB, Griem's CT is still used by a number of groups performing laboratory experiments or astrophysical observations (especially, by the latter groups) for the comparison with their experimental or observational results. In the present study we engage unexplored capabilities of the CT for *creating analytically a more accurate CT* – beyond the CT version by Griem. First, we take into account that the perturbing electrons actually do not move as free particles – in distinction to Griem's CT. This is because hydrogen (or deuterium, or tritium) atoms possess permanent electric dipole moments. Therefore perturbing electrons move in a dipole potential $V = \langle \mathbf{R} \rangle \bullet \mathbf{r}/r^3$, where $\mathbf{r}$ is the radius-vector of the perturbing electrons and $\langle \mathbf{R} \rangle$ is the mean value of the radius vector of the atomic electron. Second, Griem's definition of the so-called Weisskopf radius was not quite accurate. Third, in his book of year 1974, Griem suggested changing so-called strong collision constant without changing the Weisskopf radius, while in reality the choices of the Weisskopf radius and of the strong collision constant are interrelated. We show that the above refinements of the CT increase the electron broadening – especially for warm dense plasmas emitting H-lines. By comparison with benchmark experiments concerning the H_α line we demonstrate that the effect of the ion dynamics (neglected in any CT) seems to be smaller than previously thought, while the effect of the acceleration of perturbing electrons by the ion field in the vicinity of the radiating atom (neglected in any CT) seems to be greater than previously thought.

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1. INTRODUCTION

Physics of the Stark broadening (SB) of spectral lines in plasmas can be best understood for spectral lines of one-electron systems, such as, e.g., hydrogen atoms. (Here and below by "hydrogen atoms" and "hydrogen spectral lines" we mean atoms and spectral lines of hydrogen, deuterium, and tritium.) The theoretical importance of this research area is warranted by two reasons. First, it is a deeply fundamental problem of the simplest, two-particle bound Coulomb system immersed in a multi-particle Coulomb system of free charges (plasma) exhibiting long-range interactions – as was noted by Lisitsa [1]. Second, due to the fact that a bound two-particle Coulomb system (hydrogen atom or hydrogen-like ion) possesses a higher algebraic symmetry than its geometrical symmetry, sophisticated analytical advances can be made into the problem of the SB of spectral lines of such a system in a plasma, thus yielding a profound physical insight. There are also several practical reasons why the SB of hydrogen lines (H-lines, including deuterium and tritium lines) is especially important.

First, hydrogen isotopes (deuterium, tritium) are employed as a fuel for the energy pursuit via the controlled fusion. In magnetically-controlled fusion machines (tokamaks, stellarators, and their hybrids), spectral lines of

hydrogen isotopes are used for the experimental determination of various parameters of the edge plasmas. In the laser-controlled fusion program, H-lines of heavy dopants (added to the deuterium/tritium fuel) are utilized for the plasma diagnostics.

Second, many types of low-temperature technological discharges for plasma processing are either hydrogen-based or have an admixture of hydrogen. Therefore, shapes and shifts of H-lines in the technological discharges are a major source of the information about the plasma parameters and serve as a tool for optimizing these technologies.

Third, H-lines are used in laser-induced breakdown spectroscopy (LIBS). LIBS is a valuable technique for determining elemental composition with the ability to analyze solids, liquids and gases with little or no sample preparation.

Fourth, hydrogen is the most abundant chemical element in the Universe. Therefore, shapes and shifts of H-lines are used for deducing physical parameters in various astrophysical objects, the most important of which is the Sun. Solar activity perturbs the Earth magnitosphere and thus affects communications, oil and gas pipelines, as well as the human health. In particular, it is commonly accepted that the most powerful solar flares should involve a development of a turbulent electric field in the solar plasma. The way to detect the turbulent electric field is through the SB of highly excited Balmer lines. Increasing the theoretical accuracy of the SB through the newest advances is crucial for detecting the turbulent EF, for a better understanding of the mechanisms of the most powerful solar flares, and eventually for improving the forecast of such flares.

The most "user-friendly" are semiclassical theories of the SB of H-lines – because their results can be expressed analytically in a relatively simple form for any H-line. In the semiclassical theories the radiator is described quantally, while the perturbing charges are described classically. Both the limited-quantal theories and the semiclassical theories use the formulation, in some sense, opposite to the fully-quantal theory. Namely, the motion of the broadening particles is assumed given and one calculates the change in the wave function of the radiator.

Within the semiclassical theories, the simplest is the so-called Conventional Theory (CT) – also known as the "standard theory". In the CT, it is assumed that from the viewpoint of the radiator, the ion microfield (i.e., the electric field due to ionic perturbers) is quasistatic, while the electron microfield is treated dynamically in the so-called impact approximation [2, 3]. (The CT is frequently referred to as Griem's theory – as presented in Kepple-Griem paper [3] and in Griem's book [4].) Roughly speaking, the impact approximation considers a sequence of binary collisions of the perturbing electrons with the radiator, the collisions being completed. The CT combines the impact approximation with an approximate solution of the time-dependent Schrödinger equation (for the radiating bound electron) obtained in the second (the first non-vanishing) order of the Dirac's time-dependent perturbation theory.

A more accurate version of the collisional theory of the SB is called the unified theory. Physically, the primary distinction of the unified theory from the CT is the allowance for incomplete collisions [5, 6].

A significant analytical advance within the CT was made by Stehle and her co-workers [7,8]. For a long time it was generally accepted that within the CT or the unified theory, the Stark profile of hydrogenic spectral lines caused by the electrons at the absence of the ion microfield, is much more complicated than a superposition of Lorentzians, corresponding to Stark components of the line. Contrary to this belief, Stehle and her co-workers found that the Stark profile in this case actually reduces to a single Lorentzian and derived a simple analytical result for the Stark width of arbitrary hydrogenic spectral lines in this case. This important result was totally counter-intuitive.

Analytical advances going beyond the CT have been exact (non-perturbative – in distinction to the CT) analytical solutions of the problem – but only if all "perturbing" charges were of the same sort. The first such solution was presented by Lisitsa and Sholin within a further approximation - the binary approximation [9]. Later Derevianko and Oks [10] removed the binary assumption used by Lisitsa and Sholin and found the exact analytical solution for the most general, *multi-particle* description of the interaction of either the electron microfield or the ion microfield with the radiating atom.

The next advance in analytical theories of the SB beyond the CT was called Generalized Theory (GT). It demonstrated for the first time that the coupling of the electron and ion microfields can be strong [11, 12] – see also Oks' book [13], Chap. 4. (Sholin, Demura, and Lisitsa [14] had previously found only a weak, logarithmic coupling between the electron and ion microfields.) This *indirect coupling* (facilitated by the radiator) increases with the growth of the electron density N_e and/or the principal quantum number n, as well as with the decrease of the temperature T [11 – 13]. The GT accomplished this by going beyond the fully-perturbative description of the electron microfield used in the CT.

Despite more complicated starting formulas, the GT was developed analytically to the same level as the CT: the GT-result for the so-called "broadening function" was still expressed via elementary functions like in the CT. For this purpose, the final formulas of the GT were derived in the impact approximation, on which the CT was based. We note that the GT can be easily extended to allow for incomplete collisions: a number of fundamental results in [11] were obtained before making the impact approximation – they represent a basis of the "unified" version of the GT.

A further extension of the ideas of the GT allowed for the first time to obtain exact analytical results for the *ion-dynamical SB*. Moreover, these results were obtained not only in the binary scenario, but also for the most general, *multi-particle description* of the interaction of the ion microfield with the radiator [15].

Another development was the allowance for a strong *direct coupling* of the electron and ion microfields. This coupling results from the *acceleration of the perturbing electrons by the ion field* in the vicinity of the radiating atom. The net result is a reduction of Stark widths and shifts [16–18].

The combined theory, i.e., the combination of the GT, the ion dynamics, and the acceleration of the perturbing electrons by the ion field, practically eliminated dramatic discrepancies (up to a factor of 2) between benchmark experiments and the CT for the H-lines – see, e.g., Chapter 9 of Oks' book [13]. For brevity we call here this combined theory as EGT (Extended Generalized Theory), but keeping in mind that the effect of the acceleration of the perturbing electrons by the ion field is not based on the GT.

Griem's version of the CT presented in Kepple-Griem paper [3] is still used by a number of groups performing laboratory experiments or astrophysical observations (especially, by the latter groups) for the comparison with their experimental or observational results. The thrust of the present study was to engage unexplored capabilities of the CT for *creating analytically a more accurate CT* – beyond the CT version by Griem – and then, by comparison with benchmark experiments to figure out more precisely and unequivocally the role of the three major non-CT effects. Those are a strong indirect coupling between the electron and ion microfield (facilitated by the radiating atom), ion dynamics, and the acceleration of the perturbing electrons by the ion field.

So, in the present study we come back to the CT for H-lines (still using the impact approximation for electrons and the quasistatic approximation for ions, just as in Griem's CT) and develop a refined CT by taking into account the following*/. Hydrogen atoms possess permanent electric dipole moments, what is intimately related to the existence of an additional conserved vector quantity – the Runge-Lenz vector **A**:

$$\mathbf{A} = -\mathbf{R}/R + (\mathbf{p}x\mathbf{L} - \mathbf{L}x\mathbf{p})/(2m_e e^2). \quad (1)$$

Here **R**, **p**, **L**, e, and m_e are the radius-vector, momentum, angular momentum, charge, and mass of the atomic electron, respectively. (The definition of **A** in Landau-Lifshitz's textbook [19] differs by the sign from (1); we adopted the sign convention from Kotkin-Serbo's book [20], which was later reproduced also in Lisitsa's review [1] and in his book [21].)

The average value of the dipole moment is antiparallel to the vector **A** (see, e.g., [1, 20, 21]). Therefore perturbing electrons move in a dipole potential

*/ In this paper we use the term "CT" for any SB theory that: (A) employs the impact approximation and the perturbation theory for all components of the electron microfield; (B) neglects the ion dynamics; (C) neglects any coupling between the electron and ion microfields; (D) neglects the acceleration of the perturbing electron by the ion field in the vicinity of the radiating atom.

$$V = e^2 \langle \mathbf{R} \rangle \bullet \mathbf{r}/r^3, \quad (2)$$

where $\mathbf{r}$ is the radius-vector of the perturbing electrons and $\langle \mathbf{R} \rangle$ is the mean value of the radius- vector of the atomic electron:

$$\langle \mathbf{R} \rangle = - 3e^2 \mathbf{A}/(4|E_{at}|), \quad (3)$$

where E_{at} is the energy of the atomic electron. Hence the perturbing electrons actually do not move as free particles – in distinction to Griem's CT.

We note that Szudy and Baylis [22] considered this effect, but in frames of the so-called "old adiabatic theory" of the SB. The old adiabatic theory takes into account only the phase modulation of the atomic oscillator, but disregards the amplitude modulation and nonadiabatic effects, both playing a very important role in the SB – see, e.g., Lisitsa's review [1]. In the present paper we allow for the scattering of the perturbing electrons on the atomic electric dipole in frames of the CT, which takes into account not only the phase modulation of the atomic oscillator, but the amplitude modulation and the nonadiabatic effects. For completeness, we also note that Ostrovsky [23] considered this effect in frames of the quantal theory of the SB. Because the quantal formalism of the SB is inherently much more complicated than the semiclassical formalism of the SB, Ostrovsky presented only a sketch of the results without specific calculations of the Stark width and its comparison with the CT.

Another refinement of the CT in the present paper has to do with the fact that Griem's definition of the so-called Weisskopf radius (defined in the next section) was not quite accurate. Also, in his book [4] Griem suggested changing so-called strong collision constant (defined in the next section) without changing the Weisskopf radius, while in reality the choices of the Weisskopf radius and of the strong collision constant are interrelated: changing the strong collision constant necessitates the corresponding change of the Weisskopf radius, as shown in detail in the next sections.

We show that the above refinements of the CT are important for warm dense plasmas emitting H-lines, i.e., for plasmas of the electron densities N_e of the order of 10^{18} cm^{-3} or higher, and of the temperatures T of several eV or lower. It turns out that the above refinements of the CT increase the electron broadening compared to Griem's CT. Further, by comparison with benchmark experiments concerning the H_α line (the most intense hydrogen line in the visible range) we demonstrate the following. For warm dense plasmas of the high end of the T range and of the low end of the N_e range, where Griem's CT underestimated the width of the line, the refined CT bring the theoretical widths closer to the experimental widths. This means that the effect of the ion dynamics, which was neglected in any CT and the addition of which removes the discrepancy between the theoretical and experimental widths, seems to be actually smaller than previously thought. For warm dense plasmas of the low end of the T range and of the high end of the N_e range, where Griem's CT overestimated the width of the line, the refined CT bring the theoretical widths further away from the experimental widths. This means that in this range of N_e and T, where the ion dynamics is less important, but the effect of the acceleration of perturbing electrons by the ion field – the effect neglected in any CT, the effect reducing the widths and bringing them in agreement with the experimental widths – seems to be actually greater than previously thought.

2. OVERVIEW OF THE CONVENTIONAL THEORY (CT) WHERE PERTURBING ELECTRONS MOVE AS FREE PARTICLES

In the general case, including overlapping lines corresponding to radiative transitions between degenerate or quasidegenerate energy levels a and b, the electron impact broadening operator is defined as follows

$$\Phi_{ab} = - \int dv\, f(v)\, N_e\, v\, \sigma(v), \quad (4)$$

where the operator $\sigma(v)$ has the form:

$$\sigma(v) = \int d\rho\, 2\pi\rho\, [1 - S_a(r, v)\, S_b^*(\rho, v)]_{ang.av}. \quad (5)$$

Here v is the velocity of the perturbing electron, f(v) is the distribution of the velocities (usually assumed to be Maxwellian), ρ is the impact parameter of the perturbing electron, S_a and S_b are the corresponding scattering matrices,

the symbols * and $[\dots]_{ang.av}$ stand for the complex conjugation and the angular average, respectively. For the particular case where non-diagonal matrix elements of the Φ_{ab} are relatively small, the corresponding lineshape is a sum of Lorentzians, whose width $\gamma_{\alpha\beta}$ and shift $\Delta_{\alpha\beta}$ are equal to the negative of the real and imaginary parts of diagonal matrix elements $<\alpha|<\beta|\Phi_{ab}|\beta>|\alpha>$, respectively:

$$\gamma_{\alpha\beta} = -\,\mathrm{Re}[{}_{\alpha\beta}(\Phi_{ab})_{\beta\alpha}],\ \ \Delta_{\alpha\beta} = -\,\mathrm{Im}[{}_{\alpha\beta}(\Phi_{ab})_{\beta\alpha}]. \tag{6}$$

Here α and β correspond to upper and lower sublevels of the levels a and b involved in the radiative transition, respectively. Here and below, for any operator f, for brevity we denote its matrix elements $<\alpha|<\beta|f|\beta>|\alpha>$ as ${}_{\alpha\beta}f_{\beta\alpha}$.

Griem's CT assumes rectilinear trajectories of the perturbing electron

$$\mathbf{r}(t) = \boldsymbol{\rho} + \mathbf{v}t, \tag{7}$$

where vector $\boldsymbol{\rho}$ is directed from the radiating atom to the point of the closest approach of the perturbing electron and is perpendicular to vector $\mathbf{v}$, so that

$$r(t) = (\rho^2 + v^2t^2)^{1/2}. \tag{8}$$

Under this assumption, after calculating the scattering matrices by the standard time-dependent perturbation theory, the operator σ takes the form

$$\sigma = \int d\rho\ 2\pi\rho\ (W^2/\rho^2), \tag{9}$$

where

$$W^2 = [2\hbar^2/(3m_e{}^2v^2)][(\mathbf{R}_a{}^2 - 2\mathbf{R}_a\mathbf{R}_b{}^* + \mathbf{R}_b{}^{*2})/a_B{}^2], \tag{10}$$

a_B being the Bohr radius.

The diagonal elements of the operator $\sigma(v)$ have the physical meaning of cross-sections of so-called optical collisions, i.e., the cross-sections of collisions leading to virtual transitions inside level a between its sublevels and to virtual transitions inside level b between its sublevels, resulting in the broadening of Stark components of the H-line. According to Eq. (9), these cross-sections $<\alpha|<\beta|\sigma(v)|\beta>|\alpha>$ are expressed through diagonal elements of the operator W^2, which in the parabolic coordinates have the form (see, e.g., [1, 14]):

$${}_{\alpha\beta}(W^2)_{\beta\alpha} = [2\hbar^2/(3m_e{}^2v^2)](9/8)[n^2(n^2+q^2-m^2-1) - 4nqn`q` + n`^2(n`^2+q`^2-m`^2-1)]. \tag{11}$$

Here n and n` are the principal quantum numbers of the upper and lower levels, respectively; $q = n_1 - n_2$ and $q` = n`_1 - n`_2$ are the electric quantum numbers of the Stark sublevels α and β, respectively, expressed through the corresponding parabolic quantum numbers; m and m` are the quantum numbers of the projection of the angular momentum in the states α and β, respectively. Thus, from Eq. (9) it follows:

$${}_{\alpha\beta}(\sigma)_{\beta\alpha} = \int d\rho\ 2\pi\rho\ {}_{\alpha\beta}(W^2)_{\beta\alpha}/\rho^2. \tag{12}$$

Obviously, the right side of Eq. (12) diverges at both small and large impact parameters. This divergence is one of the primary deficiencies of the CT.

The divergence at large ρ is an intrinsic feature of the long-range Coulomb potential involved. The plasma screens out the electric field of perturbing electrons at the distances larger than the Debye radius

$$\rho_D = [T_e/(4\pi e^2N_e)]^{1/2}, \tag{13}$$

so that the upper cutoff at $\rho_{max} = \rho_D$ is more or less natural*/. In contrast, the divergence at small impact parameters is caused exclusively by the utilization of the perturbation expansion. Indeed, according to Eqs. (5) and (9), the quantity

$$[1 - S_a(\rho, v)\ S_b{}^*(\rho, v)]_{ang.av} = (W/\rho)^2 \tag{14}$$

*/ More rigorously, $\rho_{max} = \min[\rho_D, v/\Delta\omega, v/\delta\omega(F_i)]$, where $\Delta\omega$ is the detuning from the center of the line, $\delta\omega(F_i)$ is the static Stark splitting in the ion field F_i. Physically, the requirements $\rho<v/\Delta\omega$ and $\rho< v/\delta\omega(F_i)$ are the allowances for incomplete collisions and for the removal of the degeneracy by the ion field, respectively. Typically, $\min[\rho_D, v/\Delta\omega, v/\delta\omega(F_i)] = \rho_D$.

goes to infinity when the impact parameter approaches zero. This fact contradicts the unitarity of the S-matrices:

$$|1 - S_a(\rho, v)\, S_b^*(\rho, v)| = C, \quad C \le 2. \tag{15}$$

To remedy the problem, the CT uses the quantity $(W/\rho)^2$, which has a meaning of a "strength of a collision", to subdivide the collisions into "weak" and "strong" collisions as follows. Collisions having impact parameters $\rho > \rho_{min}$, where

$$_{\alpha\beta}(W^2)_{\beta\alpha} / \rho_{min}^{\ 2} = C, \tag{16}$$

are considered weak. Collisions having impact parameters $\rho < \rho_{min}$, are considered strong, so that for them the quantity $<\alpha|<\beta|W^2|\beta>|\alpha> /\rho_{min}^{\ 2}$ under the integral in Eq. (12) is substituted by the constant C, which is called a "strong collision constant". Then the Eq. (12) takes the form:

$$_{\alpha\beta}(\sigma)_{\beta\alpha} = \int_{\rho_{min}}^{\rho_{max}} d\rho\, 2\pi\rho\, _{\alpha\beta}(W^2)_{\beta\alpha} / \rho^2 + \int_{0}^{\rho_{min}} d\rho\, 2\pi\rho C. \tag{17}$$

Obviously, the 2nd integral in Eq. (17) is equal to

$$\pi\rho_{min}^{\ 2}\, C = \pi_{\alpha\beta}(W^2)_{\beta\alpha}, \tag{18}$$

where we substituted C by the left side of Eq. (16). Then Eq. (17) can be represented in the form

$$_{\alpha\beta}(\sigma)_{\beta\alpha} = 2\pi\, _{\alpha\beta}(W^2)_{\beta\alpha}\, \{\ln[\rho_{max}/\rho_{min}(C)] + 1/2\}. \tag{19}$$

The quantity $\rho_{min}(C)$, defined by Eq. (16), obviously depends on the choice of the strong collision constant $C \le 2$. Kepple and Griem [3] chose the left side of Eq. (18) to be equal to $\pi\rho_{min}^{\ 2}$, i.e., chose C = 1. Later in his book [4] on page 70, Griem changed the choice of the left side of Eq. (18) to $3\pi\rho_{min}^{\ 2}/2$, what is equivalent to choosing C = 3/2. However, under the logarithm in Eq. (19) he still kept $\rho_{min}(1)$ – as in Kepple-Griem paper [3] – what is inconsistent. Indeed, it is clear that the choice of the left side of Eq. (18), which is the choice of the value of C, affects the choice of the quantity ρ_{min} defined by Eq. (16).

Further, Eq. (16) defines the quantity ρ_{min} individually for each Stark component of the H-line. The next step in the CT is to re-define this quantity to be the same, universal value for the entire H-line. For this purpose, in the CT one averages the matrix element $_{\alpha\beta}(W^2)_{\beta\alpha}$ in Eq. (16) over the Stark sublevels in the following way.

First, the quantity

$$W_a^{\ 2} = [2\hbar^2/(3m_e^{\ 2}v^2)]<\alpha|\mathbf{R}_a^{\ 2}|\ \alpha>/a_B^{\ 2} \tag{20}$$

is averaged over the Stark sublevels of the upper level a, resulting in

$$(W_a^{\ 2})_{av} = 2\hbar^2(\mathbf{R}_a^{\ 2}/a_B^{\ 2})_{av}/(3m_e^{\ 2}v^2), \tag{21}$$

where we denoted for brevity

$$<\alpha|\mathbf{R}_a^{\ 2}|\ \alpha>_{av} = (\mathbf{R}_a^{\ 2})_{av}. \tag{22}$$

Then, the corresponding quantity $(W_b^{\ 2})_{av}$ for the lower level b is calculated. Next, the square root of the averaged matrix element $(<\alpha\ |\ <\beta|W^2|\ \beta>|\alpha>)$ is declared to be

$$[_{\alpha\beta}(W^2)_{\beta\alpha}]_{av}^{\ 1/2} = [(W_a^{\ 2})_{av}^{\ 1/2} - (W_b^{\ 2})_{av}^{\ 1/2}] \tag{23}$$

with a justification that in this form it allows for the partial cancellation of terms in $_{\alpha\beta}(W^2)_{\beta\alpha}$ when n` approaches n. Finally, the average of the square root of Eq. (16) is represented in the form

$$[(W_a^{\ 2})_{av}^{\ 1/2} - (W_b^{\ 2})_{av}^{\ 1/2}]/C^{1/2} = \rho_W, \tag{24}$$

where the average quantity $(\rho_{min})_{av}$ is denoted ρ_W and called the Weisskopf radius. More explicitly, from Eqs. (21) and (24) it follows that

$$\rho_W(C) = [2/(3C)]^{1/2}[\hbar/(m_e v)]\,[(\mathbf{R}_a^{\,2})_{av}^{\,1/2} - (\mathbf{R}_b^{\,2})_{av}^{\,1/2}]/a_B. \quad (25)$$

Then Eq. (19) is rewritten in the form:

$$_{\alpha\beta}(\sigma)_{\beta\alpha} = 2\pi\ _{\alpha\beta}(W^2)_{\beta\alpha}\ \{\ln[\rho_{max}/\rho_W(C)] + 1/2\}. \quad (26)$$

Kepple and Griem [3], while choosing C = 1, used the following expression for the Weisskopf radius

$$\hbar(n^2 - n`^2)/(m_e v) = \rho_{WG}(1) \quad (27)$$

(here and below the superscript "G" stands for "Griem"). The same expression for the Weisskopf radius was used also in Griem's book [4]. It corresponds to setting $(\mathbf{R}_a^{\,2})_{av}/a_B^{\,2} = 3n^4/2$ and $(\mathbf{R}_b^{\,2})_{av}/a_B^{\,2} = 3n`^4/2$.

However, a more accurate calculation of $(\mathbf{R}_a^{\,2})_{av}$ and $(\mathbf{R}_b^{\,2})_{av}$ yields a different result. Indeed,

$$<\alpha|\mathbf{R}_a^{\,2}|\ \alpha>/a_B^{\,2} = (9/8)n^2(n^2 + q^2 - m^2 - 1) \quad (28)$$

(see, e.g., [1, 14] or Eqs. (10) and (11)). Since $(q^2)_{av} = (m^2)_{av}$, then

$$<\alpha|\mathbf{R}_a^{\,2}|\ \alpha>_{av}/a_B^{\,2} = (9/8)n^2(n^2 - 1). \quad (29)$$

The same result can be obtained from the well-known expression for the matrix element of $\mathbf{R}_a^{\,2}$ in the spherical quantization (n, *l*, m) – see, e.g., Landau-Lifshitz's textbook [19]:

$$<n\mathit{l}m\ |\mathbf{R}_a^{\,2}|n\mathit{l}m>/a_B^{\,2} = (9/4)n^2(n^2 - \mathit{l}^2 - \mathit{l} - 1). \quad (30)$$

Indeed,

$$(<n\mathit{l}m\ |\mathbf{R}_a^{\,2}|n\mathit{l}m>)_{av}/a_B^{\,2} = (9/4)n^2\ [(1/n^2)\sum_{\mathit{l}=0}^{n-1}(n^2 - \mathit{l}^2 - \mathit{l} - 1)(2\mathit{l} + 1) = (9/8)n^2(n^2 - 1), \quad (31)$$

i.e., the same result as obtained above in the parabolic quantization.

Therefore, the leading term in $(<n\mathit{l}m\ |\mathbf{R}_a^{\,2}|n\mathit{l}m>)_{av}/a_B^{\,2}$ is $9n^4/8$ rather than the quantity $3n^4/2$ used by Griem. Substituting this more accurate result in Eq. (25) we obtain the following more accurate expression for the Weisskopf radius:

$$\rho_{WA}(C) = (3/C)^{1/2}\,\hbar(n^2 - n`^2)/(2m_e v), \quad (32)$$

(here and below the superscript "A" stands for "accurate").

Thus, in Griem's CT, Eq. (26) becomes

$$_{\alpha\beta}(\sigma)_{\beta\alpha,G} = 2\pi\ _{\alpha\beta}(W^2)_{\beta\alpha}\ \{\ln[\rho_{max}/\rho_{WG}(1)] + 1/2\} \quad (33)$$

with $\rho_{WG}(1)$ given by Eq. (27), while more accurately it should be

$$_{\alpha\beta}(\sigma)_{\beta\alpha,A} = 2\pi\ _{\alpha\beta}(W^2)_{\beta\alpha}\ \{\ln[\rho_{max}/\rho_{WA}(C)] + 1/2\} \quad (34)$$

with $\rho_{WA}(C)$ given by Eq. (32).

3. CONVENTIONAL THEORY (CT) ALLOWING FOR THE SCATTERING OF PERTURBING ELECTRONS ON THE ATOMIC ELECTRIC DIPOLE

In reality, the perturbing electrons do not pass the radiating atom as free particles. Rather, they move in the dipole potential $V = e^2<\mathbf{R}>\bullet\mathbf{r}/r^3$, as described in the Introduction. In the spherical coordinates in the **r**-space with the polar axis along the mean value $<\mathbf{R}>$ of the radius- vector of the atomic electron, the dipole potential takes the form

$$V(r, \theta) = (d\cos\theta)/r^2, \quad d = e^2|<\mathbf{R}>|, \quad (35)$$

where θ is the polar angle of the vector **r** and $<\mathbf{R}>$ is the mean value of the radius- vector of the atomic electron. In the parabolic coordinates in the **R**-space, the latter quantity is (see, e.g., Landau-Lifshitz's textbook [19]) $<\mathbf{R}> = 3nqa_B/2$, so that for the Ly-lines $d = 3n|q|e^2a_B/2$. More generally, one should use the arithmetic average of the values

of d for the upper and lower Stark sublevels – as suggested by Nienhuis [24] and used by Zsudy and Baylis [22]. Therefore, in the present paper we use the following value of d:

$$d = 3(n|q| + n`|q`|)e^2a_B/4. \quad (36)$$

The motion in a dipole potential, like the one from Eq. (35), has been studied in detail by a number of authors [25 – 27]. The primary feature of this physical system is that, in addition to the conservation of the projection M_z of the angular momentum **M** on the axis of symmetry (which is along <**R**> in our case), there exists an additional conserved quantity B:

$$B = M^2 + 2m_e d \cos\theta. \quad (37)$$

Since this quantity is conserved at any instant of time, it can be expressed through its value at $t = -\infty$ as follows

$$B = (m_e v_0 \rho_0)^2 + 2m_e d \cos\theta_0. \quad (38)$$

Here ρ_0 is the asymptotic impact parameter at $t = -\infty$ and θ_0 is the angle between <**R**> and **r**(–∞), which is the same angle as between <**R**> and $-\mathbf{v}_0$, where $\mathbf{v}_0$ is the velocity **v**(–∞) of the perturbing electron at $t = -\infty$.

Another important feature of this physical system is that it allows the separation of the radial motion from the angular motion. The radial motion occurs in an effective potential $U_{eff} = B/(2m_e r^2)$, resulting in the following time dependence of the absolute value of the radial coordinate

$$r(t) = [B/(2m_e E) + (2E/m_e)t^2]^{1/2}, \quad (39)$$

where E is the energy of the perturbing electron. Substituting B from Eq. (38) and $E = m_e v_0^2/2$ in Eq. (39), we get

$$r(t) = (\rho_{eff}^2 + v_0^2 t^2)^{1/2}, \quad (40)$$

where

$$\rho_{eff} = [\rho_0^2 + 2d \cos\theta_0/(m_e v_0^2)]^{1/2}. \quad (41)$$

Below for brevity of formulas we use v instead of v_0. After denoting

$$2d/(m_e v^2) = \rho_d^2, \quad (42)$$

Equation (41) takes the form:

$$\rho_{eff} = (\rho_0^2 + \rho_d^2 \cos\theta_0)^{1/2}. \quad (43)$$

The comparison of Eqs. (40) and (8) shows that the motion of the perturbing electron occurs with an effective impact parameter ρ_{eff} given by Eq. (41). This allow us to apply the standard effective trajectories method used in atomic physics for calculating cross-sections – see, e.g., Lebedev-Beigman's book [28], page 230. According to this method, the actual nonrectilinear trajectory is substituted by an effective rectilinear trajectory characterized by the velocity v_0 and by the effective impact parameter ρ_{eff} from Eq. (43). Then instead of Eq. (12) we have

$$_{\alpha\beta}[\sigma(\theta_0)]_{\beta\alpha} = \int d\rho_0\, 2\pi\rho_0\, {}_{\alpha\beta}(W^2)_{\beta\alpha}/\rho_{eff}^2 = \int d\rho_0\, 2\pi\rho_0\, [{}_{\alpha\beta}(W^2)_{\beta\alpha}/(\rho_0^2 + \rho_d^2 \cos\theta_0)]. \quad (44)$$

The next step is the averaging of $1/(\rho_0^2 + \rho_d^2 \cos\theta_0)]$ over the angle θ_0:

$$(1/2)\int_{-1}^{1} d(\cos\theta_0)/(\rho_0^2 + \rho_d^2 \cos\theta_0) = [1/(2\rho_d^2)]\ln[(\rho_0^2/\rho_d^2 + 1)/(\rho_0^2/\rho_d^2 - 1)]. \quad (45)$$

Now, instead of Eq. (17), we have

$$_{\alpha\beta}(\sigma)_{\beta\alpha,d} = \int_{\rho_{min}}^{\rho_{max}} d\rho_0\, 2\pi\rho_0\, [{}_{\alpha\beta}(W^2)_{\beta\alpha}/(2\rho_d^2)]\ln[(\rho_0^2/\rho_d^2 + 1)/(\rho_0^2/\rho_d^2 - 1)] + \int_0^{\rho_{min}} d\rho_0\, 2\pi\rho_0\, C, \quad (46)$$

where ρ_{min} is defined by the condition:

$$[{}_{\alpha\beta}(W^2)_{\beta\alpha}/(2\rho_d^2)]\ln[(\rho_{min}^2/\rho_d^2 + 1)/(\rho_{min}^2/\rho_d^2 - 1)] = C \quad (47)$$

(obviously, $\rho_{min} > \rho_d$). Here and below the superscript "d" in ${}_{\alpha\beta}(\sigma)_{\beta\alpha',d}$ signifies that this cross-section was obtained with the allowance for the scattering on the atomic electric dipole.

The integration over ρ_0 in Eq. (46) can be also performed analytically, yielding:

$$ {}_{\alpha\beta}(\sigma)_{\beta\alpha',d} = (\pi/2)\,{}_{\alpha\beta}(W^2)_{\beta\alpha}\{[(\rho_{max}^2/\rho_d^2)\ln[(\rho_{max}^2+\rho_d^2)/(\rho_{max}^2-\rho_d^2)] - (\rho_{min}^2/\rho_d^2)\ln[(\rho_{min}^2+\rho_d^2)/(\rho_{min}^2-\rho_d^2)]+\ln[(\rho_{max}^4-\rho_d^4)/(\rho_{min}^4-\rho_d^4)]\}+\pi C\rho_{min}^4. \quad (48)$$

After substituting the expression for the strong collision constant C from Eq. (47) in formula (48), the latter reduces to:

$$ {}_{\alpha\beta}(\sigma)_{\beta\alpha',d} = 2\pi_{\beta\alpha}(W^2)_{\beta\alpha}\{\ln[(\rho_{max}/\rho_{min})\,(\rho_{max}^4-\rho_d^4)^{1/4}/(\rho_{min}^4-\rho_d^4)^{1/4}]+[\rho_{max}^2/(4\rho_d^2)]\ln[(\rho_{max}^2+\rho_d^2)/(\rho_{max}^2-\rho_d^2)]\}. \quad (49)$$

In the limit where $\rho_{max}/\rho_{min} >> 1$, Eq. (49) simplifies to:

$$ {}_{\alpha\beta}(\sigma)_{\beta\alpha',d} = 2\pi\,{}_{\alpha\beta}(W^2)_{\beta\alpha}\,[\ln[(\rho_{max}/\rho_{min}) + 1/2 - (1/4)\ln(1-\rho_d^4/\rho_{min}^4)]. \quad (50)$$

The quantity ρ_{min} in Eqs. (49) and (50) is the solution of Eq. (47) with respect to ρ_{min}:

$$ \rho_{min} = \rho_d\,\{[\exp(2C\rho_d^2/{}_{\alpha\beta}(W^2)_{\beta\alpha}) + 1]/[\exp(2C\rho_d^2/{}_{\alpha\beta}(W^2)_{\beta\alpha}) - 1\,]\}^{1/2}. \quad (51)$$

In the limit where $C\rho_d^2/{}_{\alpha\beta}(W^2)_{\beta\alpha} >> 1$, Eq. (51) yields $\rho_{min} = [{}_{\alpha\beta}(W^2)_{\beta\alpha}/C]^{1/2}$, while in the opposite limit Eq. (51) yields $\rho_{min} = \rho_d$. However, the opposite limit does not correspond to the actual situation for any H-line, as will be shown below.

Equation (51) defines the quantity ρ_{min} individually for each Stark component of the H-line. The next step is the same as in Sect. 2: to re-define ρ_{min} to be a universal value for the entire H-line. For the average quantity $[{}_{\alpha\beta}(W^2)_{\beta\alpha})/C]^{1/2}$ we use the same result as in Sect. 2, i.e., $(3/C)^{1/2}\hbar(n^2 - n'^2)/(2m_e v)$ denoted as $\rho_{WA}(C)$ in Eq. (32). As for the quantity d that controls the value of ρ_d, by averaging the right side of Eq. (36) (where d was defined) over Stark sublevels we get $\langle d\rangle_{av} = (n^2 + n`^2)e^2a_B/4$. Substituting this into the definition of ρ_d in Eq. (42), we find:

$$ \langle\rho_d\rangle_{av} = [(n^2 + n`^2)/2]^{1/2}\,\hbar/(m_e v). \quad (52)$$

Thus, from Eqs. (51) and (52) we obtain the universal value $\langle\rho_{min}\rangle_{av}$ for the entire H-line:

$$ \langle\rho_{min}\rangle_{av} = \langle\rho_d\rangle_{av}\,\{[\exp(2\langle\rho_d\rangle_{av}^2/\rho_{WA}(C)^2) + 1]/[\exp(2\langle\rho_d\rangle_{av}^2/\rho_{WA}(C)^2) - 1\,]\}^{1/2}. \quad (53)$$

Now we come back to Eq. (49), substitute ρ_{min} by $\langle\rho_{min}\rangle_{av}$ and ρ_d by $\langle\rho_d\rangle_{av}$, and by introducing dimensionless parameters

$$ x = \langle\rho_d\rangle_{av}/\rho_{max}, \quad b = \langle\rho_d\rangle_{av}/\rho_{WA}(C) = (2C/3)^{1/2}(n^2 + n`^2)^{1/2}/(n^2 - n`^2), \quad (54)$$

we finally obtain:

$$ {}_{\alpha\beta}(\sigma)_{\beta\alpha',A,d} = 2\pi\,{}_{\alpha\beta}(W^2)_{\beta\alpha}\{\ln[(\exp(2b^2)-1)^{1/2}(1/x^4-1)^{1/4}/2^{1/2}] - b^2/2 + [1/(4x^2)]\ln[(1+x^2)/(1-x^2)]\}. \quad (55)$$

Since the parameter b in Eq. (55) is defined (by Eq. (54)) through the more accurate expression for the Weisskopf radius $\rho_{WA}(C)$, the superscript "A" is added in ${}_{\alpha\beta}(\sigma)_{\beta\alpha',A,d}$.

More importantly, the velocity v of the perturbing electrons cancelled out from the definition of the parameter b, so that the ratio $b/C^{1/2}$ is just a combination of the principal quantum numbers n and n': it takes a fixed value specific for each H-line and it does not depend on the temperature T and the electron density N_e of the plasma. Taking into account that $C \le 2$, from the definition of b in Eq. (54) it is seen that $b < 1$ always, reaching maximum values for $n` = n - 1$, i.e., for the most intense H-line of each spectral series. For example, for H_α line we get $b = 0.59\,C^{1/2}$.

The other dimensionless parameter $x = \langle\rho_d\rangle_{av}/\rho_{max}$ in Eq. (55) significantly depends on plasma parameters. In the typical case, where ρ_{max} is equal to the Debye radius ρ_D (given in Eq. (13)), the parameter x can be represented in the form

$$ x = (2e\hbar/T)[(n^2 + n`^2)N_e/m_e]^{1/2} = 2.097x10^{-11}\quad[(n^2 + n`^2)N_e]^{1/2}/T, \quad (56)$$

where in the last, practical part of Eq. (56), the temperature T is in eV and the electron density N_e is in cm^{-3}. While deriving Eq. (56), the quantity 1/v in the expression for $<\rho_d>_{av}$ (given by Eq. (52)) was substituted by its average over the Maxwell distribution $<1/v> = [2m_e/(\pi T)]^{1/2}$ – just as in Griem's CT. For warm dense plasmas emitting H-lines, the parameter x can reach values ~ 0.1 or even slightly greater.

From the ratio of the cross-sections ${}_{\alpha\beta}(\sigma)_{\beta\alpha',A,d}/{}_{\alpha\beta}(\sigma)_{\beta\alpha',A}$, where the denominator is given by Eq. (34) and the numerator – by Eq. (55), the matrix element ${}_{\alpha\beta}(W^2)_{\beta\alpha}$ cancels out, so that this ratio becomes a universal function of just two dimensionless parameters x and b applicable for any set of the five parameters N_e, T, n, n`, and C:

$$\text{ratio} = {}_{\alpha\beta}(\sigma)_{\beta\alpha',A,d}/{}_{\alpha\beta}(\sigma)_{\beta\alpha',A} = \{\ln[(\exp(2b^2)-1)^{1/2}(1/x^4-1)^{1/4}/2^{1/2}] - b^2/2 + [1/(4x^2)]\ln[(1+x^2)/(1-x^2)]\}/\{\ln[b/x] + 1/2\}. \quad (57)$$

Moreover, since the parameter x in Eq. (57) is given by Eq. (56) obtained by averaging over the Maxwell distribution of the velocities of the perturbing electrons, then the ratio in Eq. (57) is essentially the same as the ratio of widths:

$$\text{ratio} = \gamma_{\alpha\beta',A,d} / \gamma_{\alpha\beta',A}. \quad (58)$$

Here both the numerator and the denominator are defined by Eqs. (4) and (6), but with substituting ${}_{\alpha\beta}(\sigma)_{\beta\alpha',A,d}$ in Eq. (4) for calculating $\gamma_{\alpha\beta',A,d}$ and with substituting ${}_{\alpha\beta}(\sigma)_{\beta\alpha',A}$ in Eq. (4) for calculating $\gamma_{\alpha\beta',A}$. In other words, this is the ratio of widths calculated with and without the allowance for the scattering of the perturbing electrons on the atomic electric dipole, where both in the numerator and the denominator we use the more accurate expression for the Weisskopf radius ρ_{WA} given by Eq. (32).

For comparison with Griem's CT, a modification has to be made to the corresponding ratio of widths. After taking into account Griem's choice of the Weisskopf radius ρ_{WG} (given by Eq. (27)), the denominator in Eq. (57) changes to $\{\ln[b/(xC^{1/2})] + 0.356\}$, so that the corresponding ratio becomes

$$\text{ratioAtoG} = \gamma_{\alpha\beta',A,d} / \gamma_{\alpha\beta',G} =$$
$$\{\ln[(\exp(2b^2)-1)^{1/2}(1/x^4-1)^{1/4}/2^{1/2}] - b^2/2 + [1/(4x^2)]\ln[(1+x^2)/(1-x^2)]\}/\{\ln[b/(xC^{1/2})] + 0.356\}. \quad (59)$$

Figure 1 presents a three-dimensional plot of this ratio with the quantity C = 3/2 suggested on page 70 the of Griem's book [4]. It is seen that the above refinements of the CT increase the electron contribution to the width.

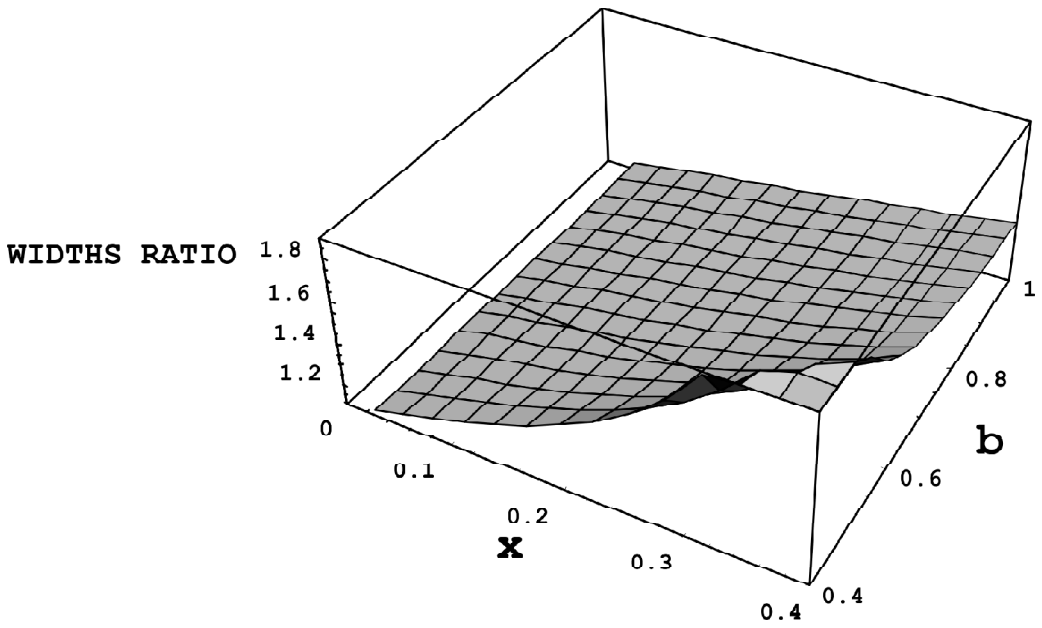

Figure 1: A three-dimensional plot of the ratio (given by Eq. (59)) of the electron impact width in the CT, refined in the present paper, with C = 3/2 to the electron impact width in Griem's CT versus dimensionless parameters x and b given by Eqs. (56) and (54), respectively.

Figure 2 presents the same ratio from Eq. (59) for the H_α line versus the dimensionless parameter x (given by Eq. (56)) for two different choices of the strong collision constant: C = 3/2 (solid curve) and C = 1 (dashed curve). In the range of $0 < x < 0.56$, where the solid curve is above the dashed curve, the relative difference between the two curves is about 15% at x = 0.4 and it diminishes toward both ends of this range.

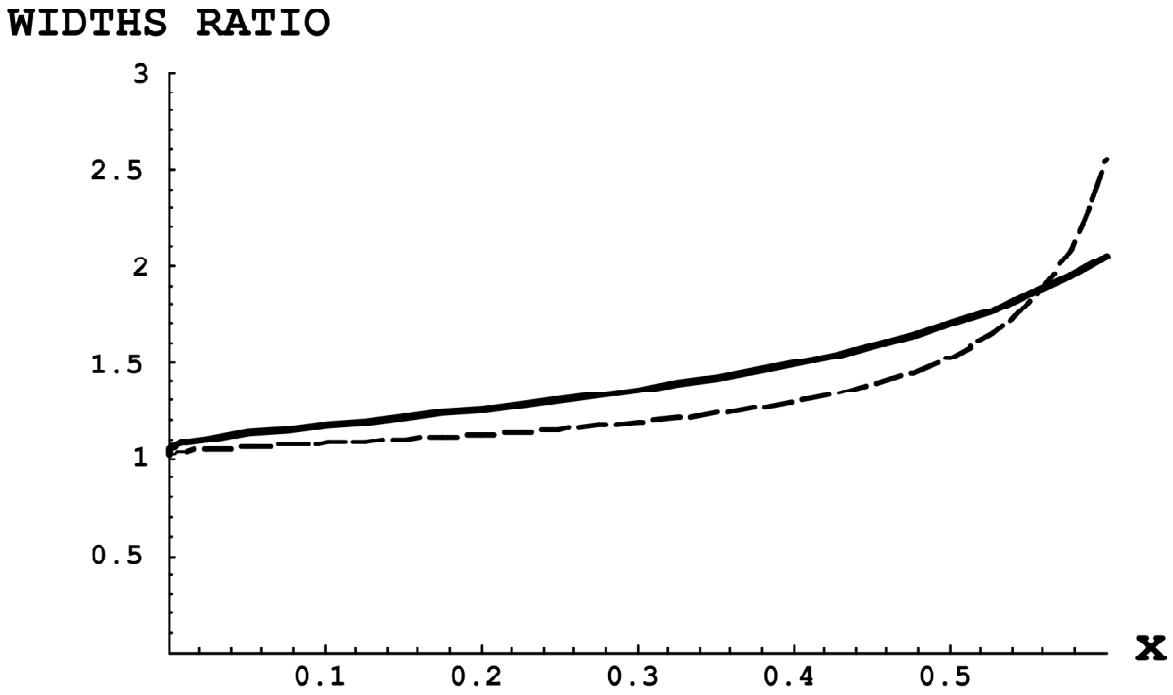

Figure 2: The ratio (given by Eq. (59)) of the electron impact width in the CT, refined in the present paper, to the electron impact width in Griem's CT, calculated for the H_α line versus the dimensionless parameter x (given by Eq. (56)) for two different choices of the strong collision constant: C = 3/2 (solid curve) and C = 1 (dashed curve).

Figures 3 and 4 present the comparison of the experimental widths of the H_α line from two different benchmark experiments with several theories. Namely, in Fig. 3 the experimental data was obtained by Kunze's group in a gas-liner pinch plasma [29], while in Fig. 4 the experimental data was obtained by Vitel's group in a flash tube plasma. In both figures the experimental widths are presented by separated dots. As for the theories, in both figures the solid curve corresponds to the refined CT from the present paper, the dotted curve – to Griem's CT, and the dashed curve – to the Extended Generalized Theory (EGT). It should be emphasized that the theoretical widths based on the refined CT, developed in the present paper, have been calculated taking into account both diagonal and nondiagonal matrix elements of the electron impact broadening operator, as well as the quasistatic broadening by ions, i.e., in the same way as in Griem's CT. We also note that the theoretical widths based on the EGT are not new results, but rather are those that had been previously calculated and presented in Oks' book [13] in Sects. 9.1 and 9.2.

The experimental data by Kunze's group [29] presented in Fig. 3 was obtained at the high end of the T range ((6 – 8) eV) and the low end of the N_e range ($(0.5 – 2.5)\times10^{-18}$ cm^{-3}). It is seen that in this range, where Griem's CT dramatically underestimated the widths compared to the experiment, the employment of the refined CT from the present paper diminished the discrepancy, though only slightly. In this range of plasma parameters, the primary reason for the discrepancy between the experiment and either one of the CT theories is the neglect of the ion dynamics. Thus, since in this range of plasma parameters, the employment of the refined CT brought the theoretical widths closer to the experimental widths, then the role of the ion dynamics seems to be smaller than previously thought. As for the EGT, which incorporated the ion dynamics using analytical results obtained within the GT formalism, it shows the best agreement with the experiment – as previously presented in Sect. 9.1 of Oks' book [13].

The experimental data by Vitel's group [14] presented in Fig. 3 was obtained at the low end of the T range ((1 – 1.5) eV) and the high end of the N_e range (up to $4x10^{-18}$ cm^{-3}). It is seen that in this range, where Griem's CT dramatically underestimated the widths compared to the experiment, the employment of the refined CT from the present paper increased the discrepancy. In this range of plasma parameters, the ion dynamics is less important and the primary reason for the discrepancy between the experiment and either one of the CT theories is the neglect of the acceleration of perturbing electrons by the ion field in the vicinity of the radiating atom: this effect diminishes the widths. Thus, since in this range of plasma parameters, the employment of the refined CT brought the theoretical widths further away from the experimental widths, then the role of the acceleration of perturbing electrons by the ion field seems to be greater than previously thought. As for the EGT, which incorporated this effect, it shows the best agreement with the experiment – as previously presented in Sect. 9.2 of Oks' book [13].

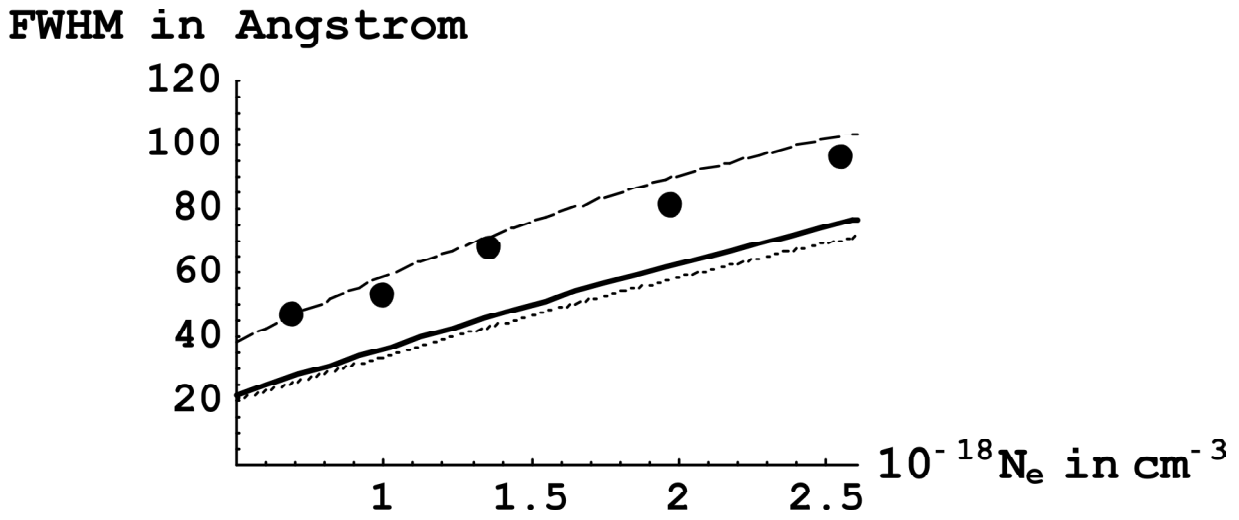

Figure 3: Comparison of the experimental widths of the H_α line (separated dots) obtained by Kunze's group in a gas-liner pinch plasma [29] at the temperatures (6 – 8) eV with the following theories: the refined CT from the present paper (solid line), Griem's CT (dotted line), the Extended Generalized Theory (dashed line).

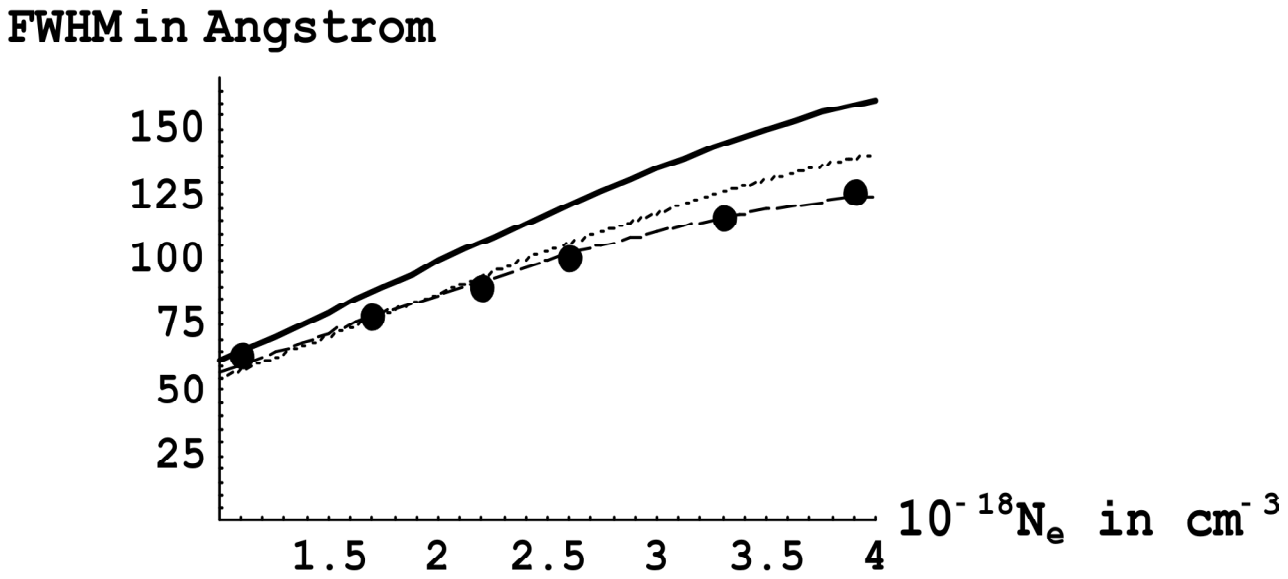

Figure 4: Comparison of the experimental widths of the H_α line (separated dots) obtained by Vitel's group in a flash tube plasma [14] at the temperatures (6 – 8) eV and the initial gas pressure 600 Torr with the following theories: the refined CT from the present paper (solid line), Griem's CT (dotted line), the Extended Generalized Theory (dashed line).

4. CONCLUSIONS

In the present study we engaged unexplored capabilities of the Conventional Theory (CT) of the Stark broadening of H-lines by electrons for *creating analytically a more accurate CT* – beyond the CT version by Griem. First, we took into account that the perturbing electrons actually do not move as free particles – in distinction to Griem's CT – but rather move in the potential of the atomic electric dipole. This is because hydrogen (or deuterium, or tritium) atoms possess permanent electric dipole moments. Second, we employed a more accurate definition of the so-called Weisskopf radius then the one used by Griem. Third, we used the value of the so-called strong collision constant suggested by Griem in his book [4], but in connection with the corresponding change of the Weisskopf radius: the choices of the Weisskopf radius and of the strong collision constant are actually interrelated, which was disregarded by Griem.

We showed that the above refinements of the CT increase the electron broadening – especially for warm dense plasmas emitting H-lines. By comparison with benchmark experiments concerning the H_α line we demonstrated that the effect of the ion dynamics (neglected in any CT) seems to be smaller than previously thought, while the effect of the acceleration of perturbing electrons by the ion field in the vicinity of the radiating atom (neglected in any CT) seems to be greater than previously thought.

We used the standard impact formalism (that implies, in particular, completed collisions) for the simplicity of the analytical results – just to get the message across and to stimulate further studies. The refined CT presented in this paper can be generalized to allow for incomplete collisions.

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