I R A M P
8(1), June 2017, pp. 41-51

ISSN: 2229-3159

Hydrogen Atoms in a Nonuniform Electric Field: Center-of-Mass Effects and their Applications

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ABSTRACT: We consider hydrogen atoms in a nonuniform electric field and study whether or not the Center-of-Mass (CM) motion and the relative motion can be separated. First, we show that in the general problem of two charges in a nonuniform electric field, the CM and relative motions, rigorously speaking, cannot be separated. Second, we use an approximate analytical method of the separation of rapid and slow subsystems to achieve a pseudoseparation of the CM and relative motions for hydrogenic atoms/ion in an arbitrary nonuniform electric field. Third, we further develop these results for the case of a hydrogen atom in the nonuniform electric field, where the field is due to the nearest (to the hydrogen atom) ion in a plasma. Fourth, we apply the results to the ion dynamical Stark broadening of hydrogen lines in plasmas. Fifth, we present specific examples of laboratory plasmas (e.g., magnetic fusion plasmas or radiofrequency discharges) and astrophysical plasmas (e.g., in atmospheres of flare stars) where the allowance for these CM effects leads to a significant increase of the width of hydrogen spectral lines.

Key words: center-of-mass effects; pseudoseparation in a nonuniform electric field; Stark broadening of hydrogen lines in plasmas; magnetic fusion; radiofrequency discharges; flare stars

1. INTRODUCTION

It is well-known that for hydrogenic atoms/ions in a uniform magnetic field, the Center-of-Mass (CM) motion and the relative (internal) motion are coupled and, rigorously speaking, cannot be separated – see, e.g., papers [1-3] and references therein. For hydrogen atom it is possible to achieve a pseudoseparation leading to a Hamiltonian for the relative motion that still depends on a CM integral of the motion called pseudomomentum [3].

As for hydrogenic atoms/ions in a uniform electric field, it is well-known that the CM and relative motions can be separated rigorously (exactly) – see, e.g., [4]. As for hydrogenic atoms/ions in a nonuniform electric field, there seem to be nothing about the separation (or non-separation) of the CM and relative motions in the literature, to the best of our knowledge.

In the present paper we study this issue for hydrogenic atoms/ions in a nonuniform electric field. First, we show that in the general problem of two charges in a nonuniform electric field, the CM and relative motions, rigorously speaking, cannot be separated. Second, we use an approximate analytical method of the separation of rapid and slow subsystems to achieve a pseudoseparation of the CM and relative motions for hydrogenic atoms/ion in an arbitrary nonuniform electric field. Third, we further develop these results for the case of a hydrogen atom in the nonuniform electric field, where the field is due to the nearest (to the hydrogen atom) ion in a plasma. Fourth, we apply the results to the ion dynamical Stark broadening of hydrogen lines in plasmas. Fifth, we present specific examples of laboratory and astrophysical plasmas where the allowance for these CM effects leads to a significant increase of the width of hydrogen spectral lines.

2. GENERAL CASE OF THE PSEUDOSEPARATION OF THE CENTER-OF-MASS AND RELATIVE MOTIONS IN A NONUNIFORM ELECTRIC FIELD

We consider a system of two charges e_1 and e_2 of masses m_1 and m_2, respectively, in a nonuniform electric field. The Lagrangian of the system is

$$L = [m_1(d\mathbf{r}_1/dt)^2 + m_2(d\mathbf{r}_2/dt)^2]/2 - e_1e_2/|\mathbf{r}_2 - \mathbf{r}_1| - e_1\varphi(\mathbf{r}_1) - e_2\varphi(\mathbf{r}_2), \quad (1)$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are radii-vectors of charges e_1 and e_2, respectively and φ is the potential of the nonuniform electric field. After the substitution

$$\mathbf{R} = (m_1\mathbf{r}_1 + m_2\mathbf{r}_2)/(m_1 + m_2), \qquad \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1, \quad (2)$$

so that $\mathbf{R}$ and $\mathbf{r}$ are the coordinates related to the CM motion and the relative motion, respectively, the Lagrangian takes the form

$$L(\mathbf{R}, \mathbf{r}) = L_{CM}(\mathbf{R}) - U(\mathbf{R}, \mathbf{r}) + L_r(\mathbf{r}), \quad (3)$$

where

$$L_{CM}(\mathbf{R}) = (m_1 + m_2)(d\mathbf{R}/dt)^2/2 - (e_1 + e_2)\varphi(\mathbf{R}) \quad (4)$$

is the Langrangian of the CM,

$$L_r(\mathbf{r}) = \mu(d\mathbf{r}/dt)^2/2 - e_1e_2/r \quad (5)$$

is the Lagrangian of the relative motion, and

$$U(\mathbf{R}, \mathbf{r}) = \mu(e_1/m_1 - e_2/m_2)\mathbf{rF}(\mathbf{R}) \quad (6)$$

is the coupling of the CM and relative motions. Here

$$\mu = m_1m_2/(m_1 + m_2) \quad (7)$$

is the reduced mass of the two particles, and

$$\mathbf{F}(\mathbf{R}) = -d\varphi(\mathbf{R})/d\mathbf{R} \quad (8)$$

is a nonuniform electric field (in the expansion of the electric potential we disregarded terms higher than the dipole one). In Eq. (6) and below, for any two vectors **A** and **B**, the notation **AB** stands for the scalar product (also known as the dot-product) of the two vectors.

The Hamiltonian, corresponding to the Langrangian from Eq. (3), has the form

$$H = H_{CM}(\mathbf{R}, \mathbf{P}) + U(\mathbf{R}, \mathbf{r}) + H_r(\mathbf{r}, \mathbf{p}), \quad (9)$$

where

$$H_{CM}(\mathbf{R}, \mathbf{P}) = P^2/[2(m_1 + m_2)] + (e_1 + e_2)\varphi(\mathbf{R}) \quad (10)$$

is the Hamiltonian of the CM, **P** being the momentum of the CM motion, and

$$H_r(\mathbf{r}, \mathbf{p}) = p^2/(2\mu) + e_1e_2/r \quad (11)$$

is the Hamiltonian of the relative motion, **p** being the momentum of the relative motion.

Thus, the above equations show that at the presence of a nonuniform electric field, the CM motion and the relative motion are coupled (by U(**R**, **r**) from Eq. (6)) and therefore, rigorously speaking, cannot be separated. However, in the case where $m_1 << m_2$, the CM and relative motions can be separated by using the approximate analytical method of separating rapid and slow subsystems: in this case, the characteristic frequency of the relative motion is much greater than the characteristic frequency of the CM motion, so that the former and the latter are the rapid and slow subsystems, respectively. Below are the details of this method that can be found, e.g., in [5].

The first step is to freeze the coordinates **R** of the slow subsystem and to solve for the motion of the rapid subsystem characterized by the truncated Hamiltonian

$$H_{tr} = H_r(\mathbf{r}, \mathbf{p}) + U(\mathbf{R}, \mathbf{r}) = p^2/(2\mu) + e_1e_2/r + \mu(e_1/m_1 - e_2/m_2)\mathbf{rF}(\mathbf{R}), \quad (12)$$

where **R** is treated as a fixed parameter rather than as the dynamical variable. In the situation where the charges e_1 and e_2 are of the opposite sign (say, for definiteness $e_1 < 0$ and $e_2 > 0$), this becomes the Hamiltonian of a hydrogenic atom/ion in a "uniform" electric field.

By treating the last term in Eq. (12) in the first order of the perturbation theory, one obtains the following expression for the energy of the relative motion, i.e., the rapid subsystem (see, e.g., the textbook [6])

$$E(\mathbf{R}) = -\mu e_1^2e_2^2/(2n^2\hbar^2) + \mu(e_1/m_1 - e_2/m_2)\langle\mathbf{r}\rangle\mathbf{F}(\mathbf{R}) = \quad (13)$$

$$-\mu e_1^2e_2^2/(2n^2\hbar^2) - (3n^2\hbar^2/2)[1/(m_1e_2) + 1/(m_2|e_1|)]\,\mathbf{AF}(\mathbf{R}),$$

where there was used the well-known relation between the mean value $\langle\mathbf{r}\rangle$ of the radius-vector and the Runge-Lenz vector **A** (see, e.g., [7, 8]):

$$\langle\mathbf{r}\rangle = -3e_1e_2\mathbf{A}/|E_0|, \qquad E_0 = -\mu e_1^2e_2^2/(2n^2\hbar^2). \quad (14)$$

Here and below n is the principal quantum number.

By choosing the z-axis along the Runge-Lenz vector **A**, we rewrite Eq. (13) in the form

$$E(\mathbf{R}) = -\mu e_1^2e_2^2/(2n^2\hbar^2) - (3n|q|\hbar^2/2)[1/(m_1e_2) + 1/(m_2|e_1|)]\,F(\mathbf{R})\cos[\theta(\mathbf{R})], \quad (15)$$

where $\theta(\mathbf{R})$ is the polar angle of the vector $\mathbf{F}(\mathbf{R})$ and q is the electric quantum numbers ($q = n_1 - n_2$, where n_1 and n_2 are the parabolic quantum numbers).

The second step of the analytical method of separating rapid and slow subsystems is to proceed to the slow subsystem (the CM motion), for which $E(\mathbf{R})$ from Eq. (15) will play the role of an effective potential. The effective Hamiltonian $H_{\mathrm{CM,eff}}(\mathbf{R}, \mathbf{P})$ for the CM motion becomes (the first, **R**-independent term in E(**R**) has been omitted because it does not affect the CM motion)

$$H_{\mathrm{CM,eff}}(\mathbf{R}, \mathbf{P}) = P^2/[2(m_1+m_2)]+(e_1+e_2)\varphi(\mathbf{R}) -(3n|q|\hbar^2/2)[1/(m_1e_2) +1/(m_2|e_1|)]\,F(\mathbf{R})\cos[\theta(\mathbf{R})] \quad (16)$$

Thus, the application of this analytical method allowed the pseudoseparation of the CM motion and the relative motion for any two oppositely charged particles of significantly different masses in a nonuniform electric field.

In the particular case of hydrogen atoms one has

$$e_1 = e, \; e_2 = -e, \qquad \mu = m_em_p/(m_e + m_p), \quad (17)$$

where $e > 0$ is the electron charge, m_e and m_p are the electron and proton masses, respectively. Then Eq. (16) simplifies to

$$H_{\mathrm{CM,eff}}(\mathbf{R}, \mathbf{P}) = P^2/(2m) - [3n|q|\hbar^2/(2\mu e)]\,\mathrm{F}(\mathbf{R})\cos[\theta(\mathbf{R})], \qquad m = (m_e + m_p). \quad (18)$$

3. ANALYTICAL SOLUTION FOR THE CENTER-OF-MASS MOTION OF A HYDROGEN ATOM IN THE FIELD OF THE NEAREST ION AND ITS APPLICATION TO THE DYNAMICAL STARK BROADENING OF HYDROGEN LINES IN LABORATORY AND ASTROPHYSICAL PLASMAS

Now we consider the situation where the nonuniform electric field is due to the nearest (to the hydrogen atom) ion of the positive charge Ze and mass m_i in a plasma located at the distance **R** from the hydrogen atom. Then the Hamiltonian from Eq. (18) can be rewritten as

$$H_{\mathrm{CM,eff}}(\mathbf{R}, \mathbf{P}) = P^2/(2m) - (D/R^2)\cos\theta, \qquad D = [3n|q|\hbar^2/(2i)]\,Z, \quad \cos\theta = \mathbf{AR}/\mathrm{AR}. \quad (19)$$

This Hamiltonian represents a particle of mass m in the dipole potential. Since this particle is relatively heavy ($m >> m_e$), its motion can be described classically and the corresponding classical solution is well-known – see, e.g., paper [9]. For this physical system, the radial motion can be exactly separated from the angular motion resulting in the following radial equation:

$$m[R(dR/dt) + (dR/dt)^2] = E_{CM} \tag{20}$$

where E_{CM} is the total energy of the particle. This equation allows the following exact general solution:

$$R(t) = (2E_{CM}t^2/m + 2R_0v_0t + R_0^2)^{1/2}, \quad R_0 = R(0), \quad v_0 = (dR/dt)_{t=0}. \tag{21}$$

It is well-known that in plasmas of relatively low electron densities N_e, the Stark broadening of the most intense hydrogen lines, i.e., the lines corresponding to the radiative transitions between the levels of the low principal quantum numbers (such as, e.g., Ly-alpha, Ly-beta, H-alpha, etc.), is dominated by the ion dynamical broadening – see, e.g., publications [10-16]. The corresponding validity condition is presented in Appendix. In the so-called "conventional theory" of the dynamical Stark broadening (also known as the "standard theory") [17-20], the relative motion within the pair "radiator – perturber" was assumed to occur along a straight line – as for a *free motion* (in our case the radiator is a hydrogen atom and the perturber is the perturbing ion).

However, from the preceding discussion it follows that in the more advanced approach, the relative motion within the pair "radiator-perturber" should be treated as the motion in the dipole potential – $(D/R^2)\cos\theta$, as seen from Eq. (19). The relevant setup of the problem is to choose the instant $t = 0$ as the instant of the smallest distance (the closest approach) within the pair "radiator-perturber". Then $v_0 = v_0 = (dR/dt)_{t=0} = 0$, so that Eq. (21) simplifies to

$$R(t) = (2E_{CM}t^2/m + R_0^2)^{1/2}. \tag{22}$$

The energy E_{CM} can be represented in the form

$$E_{CM} = P_0^2/(2m) - (D/R_0^2)\cos\theta_0, \quad P_0 = P(0), \quad \theta_0 = \theta(0). \tag{23}$$

By considering the motion within the pair "radiator-perturber" in the reference frame where the perturbing ion is at rest, so that $P_0 = mV_0$, where V_0 is the relative velocity within the pair "radiator-perturber" at $t = 0$, the energy E_{CM} can be rewritten as

$$E_{CM} = mV_0^2/2 - (D/R_0^2)\cos\theta_0. \tag{25}$$

Then Eq. (22) becomes

$$R(t) = \{[V_0^2 - 2D\cos\theta_0/(mR_0^2)]t^2 + R_0^2\}^{1/2}. \tag{26}$$

By introducing the effective velocity

$$V_{eff}(R_0, \theta_0) = [V_0^2 - 2D\cos\theta_0/(mR_0^2)]^{1/2}, \tag{27}$$

we can make Eq. (26) to be formally equivalent to the usual case of the rectilinear trajectories:

$$R(t) = \{[V_{eff}(R_0, \theta_0)]^2t^2 + R_0^2\}^{1/2}. \tag{28}$$

Now we consider a radiative transition between hydrogen energy levels a and b. In the general case, the ion dynamical broadening operator Φ_{ab} is defined as follows (by analogy with the electron dynamical broadening operator defined, e.g., in paper [17]):

$$\Phi_{ab}(t) = -\int dV_0\, f(V_0)\, N_i\, V_0 \langle\sigma(V_0, \theta_0, t)\rangle_{\theta_0}. \tag{29}$$

Here $\langle\ldots\rangle_{\theta_0}$ denotes the averaging over the angle θ_0, and the operator $\sigma(V_0, \theta_0, t)$ has the form:

$$\sigma(V_0, \theta_0, t) = \int dR_0\, 2\pi R_0\, [1 - U^{(R_0, V_0, \theta_0)}{}_a(t, 0)\, U^{(R_0, V_0, \theta_0)}{}_b{}^*(t, 0)]_{ang.av}. \tag{30}$$

Here N_i is the ion density, $f(V_0)$ is the distribution of the velocities (usually assumed to be Maxwellian), ρ is the impact parameter of the perturbing ion, U_a and U_b are the corresponding time-evolution operators, the symbols * and $[\ldots]_{ang.av}$ stand for the complex conjugation and the angular average, respectively. If the time t would be considered as a parameter, then the diagonal elements of the operator $\sigma(V_0, t)$ would 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 hydrogen spectral line.

By using the trajectories from Eq. (26) and averaging over the polar angle θ_0, one can obtain the evolution operators and then the ion dynamical broadening operator with the allowance for the effect of the CM motion. However, in this general case, the results cannot be obtained analytically.

Therefore, for obtaining the final results analytically (which should help getting the message across in the simple form), we now employ the so-called impact approximation and substitute the evolution operators by the corresponding scattering matrices (see, e.g., papers [18, 19] or books [16, 20]):

$$\Phi_{ab} = -\int dV_0\, f(V_0)\, N_i\, V_0 < \sigma(V_0, \theta_0)>_{\theta o}, \tag{31}$$

$$\sigma(V_0, \theta_0) = \int dR_0\, 2\pi R_0\, [1 - S_a(R_0, V_0, \theta_0)\, S_b^*(R_0, V_0, \theta_0)]_{ang.av}. \tag{32}$$

In the case where non-diagonal matrix elements of the Φ_{ab} are relatively small, the lineshape is a sum of Lorentzians, whose width $\gamma_{\alpha\beta}$ and shift $\Delta_{\alpha\beta}$ are equal (apart from the sign) to the real and imaginary parts of diagonal matrix elements $<\alpha|<\beta|\Phi_{ab}|\beta>|\alpha>$, respectively:

$$\gamma_{\alpha\beta} = -\,\mathrm{Re}[{}_{\alpha\beta}(\Phi_{ab})_{\beta\alpha}], \qquad \Delta_{\alpha\beta} = -\,\mathrm{Im}[{}_{\alpha\beta}(\Phi_{ab})_{\beta\alpha}]. \tag{33}$$

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

As we calculate the scattering matrices by the standard time-dependent perturbation theory, we obtain the following expression for the operator σ

$$\sigma(R_0, V_0, \theta_0) = \int dR_0\, 2\pi R\, [K^2 Q(R_0, V_0, \theta_0)/R_0^2]. \tag{34}$$

Here

$$Q(R_0, V_0, \theta_0) = 2\hbar^2/[3\mu^2 V_{eff}(R_0, \theta_0)^2] = Q_0/[1 - 2D\cos\theta_0/(mV_0^2 R_0^2)],\ Q_0 = 2Z^2\hbar^2/(3\mu^2 V_0^2), \tag{35}$$

and

$$K^2 = K_a^2 + K_{interf} + K_b^2,\ K_a^2 = \mathbf{r}_a^2/a_B^2,\ K_{interf} = -2\mathbf{r}_a\mathbf{r}_b^*/a_B^2,\quad K_b^2 = \mathbf{r}_b^{*2}/a_B^2,\ a_B = \hbar^2/(\mu e^2), \tag{36}$$

where a_B is the Bohr radius, K_{interf} represents the so-called interference term. In the conventional theory [18-20], in Eq. (35) instead of $V_{eff}(R_0, \theta_0)$, it would be V_0^2.

The next step is the averaging of $1/V_{eff}(R_0, \theta_0)^2$ in Eq. (35) over the angle θ_0:

$$(1/2)\int_{-1}^{1} d(\cos\theta_0)/[V_0^2 - 2D\cos\theta_0/(mR_0^2)] = [R_0^2/(2R_D^2 V_0^2)]\ln[(R_0^2 + R_D^2)/(R_0^2 - R_D^2)], \tag{37}$$

where

$$R_D = [2D/(mV_0^2)]^{1/2}, \tag{38}$$

so that the quantity $Q(R_0, \theta_0)$ after the averaging over θ_0 becomes

$$Q(R_0) = [Q_0 R_0^2/(2R_D^2)]\ln[(R_0^2 + R_D^2)/(R_0^2 - R_D^2)] \tag{39}$$

with Q_0 defined in Eq. (35).

The way the quantity D (entering Eq. (38)) was defined in Eq. (19) as $D = [3n|q|\hbar^2/(2\mu)]\ Z$ is valid only for the Lyman lines. For all other hydrogen lines one should use the arithmetic average of the values of D for the upper and lower Stark sublevels – as suggested in the similar case in paper [21] and used in paper [22]. Therefore, in the present paper for all other hydrogen lines we use the following value of D

$$D = 3(n|q| + n'|q'|)Ze^2a_B/4, \tag{40}$$

where the quantum numbers with the prime symbol and without it relate to the lower and upper levels, respectively.

The next step is the averaging over R_0. The integral over R_0 in Eq. (34) has a weak, logarithmic divergence at both small and large impact parameters – just like in the conventional theory [17-20]. Therefore, as in the conventional theory, we subdivide collisions into "weak" ($R_0 > R_{min}$) and "strong" ($R_0 < R_{min}$), and introduce also the upper cutoff R_{max} (just as in the conventional theory) discussed later. Then the diagonal elements of the cross-section of optical collisions can be represented in the form

$$_{\alpha\beta}(\sigma)_{\beta\alpha,D} = \int_{R\min}^{R\max} dR_0\, 2\pi R_0\, [_{\alpha\beta}(K^2)_{\beta\alpha} Q(R_0)/R_0^2)] + \int_0^{R\min} dR_0\, 2\pi R_0\, C, \tag{41}$$

where R_{min} is defined by the condition:

$$_{\alpha\beta}(K^2)_{\beta\alpha}\, Q(R_{min})/R_{min}^{\ 2} = _{\alpha\beta}(K^2)_{\beta\alpha}\, [Q_0/(2R_D^{\ 2})] \ln[(R_{min}^{\ 2} + R_D^{\ 2})/(R_{min}^{\ 2} - R_D^{\ 2})] = C \tag{42}$$

(naturally, $R_{min} > R_D$). 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 CM motion. The constant C in Eq. (42) is called "strong collision constant" in the conventional theory. It arises from the preservation of the unitarity of the S-matrices:

$$|1 - S_a(R_0, V_0, \theta_0)\, S_b^*(R_0, V_0, \theta_0)| = C, \quad C \le 2\ . \tag{43}$$

For example, according to Griem book [20], page 43, his choice was C = 3/2. More details can be found in paper [23]*/.

As for the upper cutoff R_{max}, following the conventional theory we choose it as the Debye radius

$$R_{max} = R_{Debye} = [T/(4\pi e^2 N_e)]^{1/2}, \tag{44}$$

(though more rigorously, it should have been $R_{max} = \min(R_{Debye}, V_0/\Delta\omega)$, where $\Delta\omega$ is the detuning from the center of the spectral line; physically, the requirements $R_{max} < V_0/\Delta\omega$ being the allowance for incomplete collisions).

By integrating analytically over R_0 in Eq. (41) and substituting into the result the expression for the strong collision constant C from Eq. (42) we obtain:

$$_{\alpha\beta}(\sigma)_{\beta\alpha,D} = 2\pi\, _{\alpha\beta}(K^2)_{\beta\alpha} Q_0 \{\ln[(R_{max}^{\ 4} - R_D^{\ 4})^{1/4}/(R_{min}^{\ 4} - R_D^{\ 4})^{1/4}] + [R_{max}^{\ 2}/(4R_D^{\ 2})] \ln[(R_{max}^{\ 2} + R_D^{\ 2})/(R_{max}^{\ 2} - R_D^{\ 2})]\}. \tag{45}$$

The boundary R_{min} between the weak and strong collisions in Eq. (45) is the solution of Eq. (42) with respect to R_{min}:

$$R_{min} = R_D\, \{[\exp(2CR_D^{\ 2}/\, _{\alpha\beta}(K^2)_{\beta\alpha} Q_0) + 1]/[\exp(2CR_D^{\ 2}/\, _{\alpha\beta}(K^2)_{\beta\alpha} Q_0) - 1\ ]\}^{1/2}. \tag{46}$$

The next step is the averaging of several quantities from the above equations over Stark sublevels of the upper and lower levels, so that each of these quantities will have the unique value for the particular hydrogen spectral line. First, the square root of the averaged matrix element ($<\alpha|<\beta|K^2|\beta>|\alpha>$) is asserted to be

*/ On page 43 of book [20], Griem explicitly chose 3/2 for the quantity $|1 - S_a(R_0, V_0, \theta_0)\, S_b^*(R_0, V_0, \theta_0)|$ that we denoted as C. To avoid any confusion we note that what Griem called "strong collision term" was C/2. The extra factor 1/2 arises from the following integral for the strong collision term:

$$(1/\rho_{min}^{\ 2}) \int_0^{\rho_{min}} d\rho\ \rho C = C/2.$$

$$[{}_{\alpha\beta}(K^2)_{\beta\alpha}]_{av}^{1/2} = [{}_{\alpha}(K_a^2)_{\alpha}^{1/2} - {}_{\beta}(K_b^2)_{\beta}^{1/2}]_{av} \quad (47)$$

following the conventional theory justification [20] that in this form it allows for the partial cancellation of terms in ${}_{\alpha\beta}(W^2)_{\beta\alpha}$ when the principal quantum number n‘ of the lower level is close to the principal quantum number n of the upper level. The diagonal elements of the operators K_a^2 and K_b^2 have the following form in the parabolic coordinates (see, e.g. [7, 24])

$${}_{\alpha}(K_a^2)_{\alpha} = (9/8)n^2(n^2 + q^2 - m^2 - 1), \quad {}_{\beta}(K_b^2)_{\beta} = (9/8)n'^2(n'^2 + q'^2 - m'^2 - 1)]. \quad (48)$$

The averaging over Stark sublevels (since $(q^2)_{av} = (m^2)_{av}$) results in the following leading term in the quantity $[{}_{\alpha\beta}(K^2)_{\beta\alpha}]_{av}^{1/2}$:

$$[{}_{\alpha\beta}(K^2)_{\beta\alpha}]_{av} = (9/8)(n^2 - n'^2). \quad (49)$$

We mention that the same result (49) can be obtained after the corresponding averaging in the spherical quantization.

We denote

$$R_{WA}(C) = \{[{}_{\alpha\beta}(K^2)_{\beta\alpha}]_{av}\, Q_0/C\}^{1/2} = (3/C)^{1/2}(n^2 - n'^2)\hbar Z/(2\mu V_0). \quad (50)$$

This quantity has the meaning of the so-called Weisskopf radius: it is defined here more accurately than in the conventional theory by Griem [20] (which is why here and below the superscript “A” stands for “accurate”). The next quantity to be averaged over Stark sublevels of the upper and lower levels, so that it will have the unique value for the particular hydrogen spectral line, is the quantity D from Eq. (40). The result reads:

$$\langle D\rangle_{av} = (n^2 + n'^2)Ze^2a_B/4. \quad (51)$$

After substituting this into the definition of R_D in Eq. (38), we obtain:

$$\langle R_D\rangle_{av} = [(n^2 + n'^2)Z/2]^{1/2}\, \hbar/(\mu V_0). \quad (52)$$

Thus, from Eqs. (46), (50), and (52), we get the unique value $\langle R_{min}\rangle_{av}$ for the entire hydrogen spectral line:

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

As the last step we substitute R_{min} by $\langle R_{min}\rangle_{av}$ and R_D by $\langle R_D\rangle_{av}$ in Eq. (45), and also introduce dimensionless parameters

$$w = \langle R_D\rangle_{av}/R_{max}, \qquad b = \langle R_D\rangle_{av}/R_{WA}(C) = [2C/(3Z)]^{1/2}(n^2 + n'^2)^{1/2}/(n^2 - n'^2), \quad (54)$$

By doing so, we finally obtain:

$${}_{\alpha\beta}(\sigma)_{\beta\alpha,A,D} = 2\pi\, {}_{\alpha\beta}(K^2)_{\beta\alpha}Q_0\{\ln[(\exp(2b^2) - 1)^{1/2}(1/w^4 - 1)^{1/4}/2^{1/2}] - b^2/2 + [1/(4w^2)]\ln[(1+w^2)/(1-w^2)]\}, \quad (55)$$

where Q_0 was defined in Eq. (35) and

$${}_{\alpha\beta}(K^2)_{\beta\alpha} = (9/8)[n^2(n^2 + q^2 - m^2 - 1) - 4nqn'q' + n'^2(n'^2 + q'^2 - m'^2 - 1)]. \quad (56)$$

From Eq. (54) it is seen that the ratio $Z^{1/2}b/C^{1/2}$ is just a combination of the principal quantum numbers n and n‘ specific for each hydrogen spectral line: it is independent of the temperature T and of the electron density N_e of the plasma. Since the strong collision constant $C \le 2$, it follows from Eq. (54) that $b < 1$ always. It reaches maximum values for $n' = n - 1$, i.e., for the most intense hydrogen spectral line of each spectral series. Here are examples for the case where the charge of the perturbing ions is $Z = 1$. For the Balmer-alpha line (H_α) we get $b = 0.59\, C^{1/2}$. For the Paschen-alpha, Brackett-alpha, and higher alpha lines, the ratio $b/C^{1/2}$ rapidly approaches $1/3^{1/2} = 0.58$. For the Lyman lines the expression for the ratio $b/C^{1/2}$ should be $2/(3^{1/2}n)$ instead of Eq. (54), so that for the Lyman-alpha line one gets $b/C^{1/2} = 1/3^{1/2}$ since $n = 2$.

The other dimensionless parameter $w = \langle R_D\rangle_{av}/R_{max}$, which enters Eq. (55), significantly depends on plasma parameters. In the most frequent case, where R_{max} is equal to the Debye radius R_D (given in Eq. (38)), the parameter w can be expressed as follows

$$w = [2e\hbar/(\mu T)][(n^2 + n'^2)Zm_r N_e]^{1/2} = 8.99\text{x}10^{-10}[(n^2 + n'^2)ZN_e m_r/m_p\ ]^{1/2}/T, \quad (57)$$

where

$$m_r = (m_e + m_p)m_i / (m_e + m_p + m_i). \quad (58)$$

In the utmost right part of Eq. (57), the temperature T is in eV and the electron density N_e is in cm^{-3}. While deriving Eq. (56), the quantity $1/V_0$ in the expression for $<R_D>_{av}$ (given by Eq. (52)) was substituted by its average over the Maxwell distribution $<1/V_0> = [2m_r/(\pi T)]^{1/2}$ – just as in the conventional theory [20]. For the Lyman-lines the expression for w should be modified to

$$w = [e\hbar n/(\mu T)](2m_r ZN_e)^{1/2} = 1.27\text{x}10^{-9} n[ZN_e m_r/\ m_p\ ]^{1/2}/T, \quad (59)$$

For presenting the effect of the CM motion in the universal form, it is convenient to introduce the ratio of the cross-section ${}_{\alpha\beta}(\sigma)_{\beta\alpha',A,D}$ to the corresponding cross-section ${}_{\alpha\beta}(\sigma)_{\beta\alpha' G}$ from the conventional theory by Griem [20]. Since the parameter w in Eq. (57) was obtained by averaging over the Maxwell distribution of the velocities, then the ratio of the cross-sections is essentially the same as the ratio of widths $\gamma_{\alpha\beta',A,D}/\gamma_{\alpha\beta',G}$:

$$\text{ratio} = {}_{\alpha\beta}(\sigma)_{\beta\alpha',A,D}/{}_{\alpha\beta}(\sigma)_{\beta\alpha' G} = \gamma_{\alpha\beta',A,D}/\gamma_{\alpha\beta' G} = \quad (60)$$

$$\{\ln[(\exp(2b^2) - 1)^{1/2}(1/w^4 - 1)^{1/4}/2^{1/2}] - b^2/2 + [1/(4w^2)]\ln[(1+w^2)/(1-w^2)]\}/\{\ln[b/(wC^{1/2})] + 0.356\}.$$

The matrix element ${}_{\alpha\beta}(W^2)_{\beta\alpha}$ cancels out from this ratio, so that it becomes indeed a universal function of just two dimensionless parameters w and b applicable for any set of the five parameters N_e, T, n, n', and C.

Below we provide numerical examples for some laboratory and astrophysical plasmas where the allowance for the CM motion significantly affects the ion dynamical Stark width. The first example is edge plasmas of magnetic fusion machines (such as, e.g., tokamaks), characterized by the electron density $N_e = (10^{14} - 10^{15})$ cm^{-3} and the temperature of one or few eV (see, e.g., review [25]). For these plasma parameters, the Stark broadening of the most intense hydrogen spectral lines (Ly-alpha, Ly-beta, H-alpha, etc.) can be dominated by the ion dynamical broadening (see, e.g., [10-16]).

The second example is plasmas in the atmospheres of flare stars. They are characterized by practically the same range of plasma parameters as the edge plasmas of magnetic fusion machines – see, e.g., book [26] and paper [27].

For both the edge of magnetic fusion machines and the atmospheres of flare stars, for the $H_á$ line emitted from a hydrogen plasma at $N_e = 5\text{x}10^{14}$ cm^{-3} and $T = 1$ eV, the ratio from Eq. (60) yields 1.19 for $C = 2$ and 1.13 for $C = 3/2$. Figure 1 presents this ratio (for the H_α line emitted from a hydrogen plasma) versus the electron density N_e at $T = 1$ eV for $C = 2$ (solid line) and for $C = 3/2$ (dashed line). It is seen that the allowance for the CM motion increases the ion dynamical Stark width of the $H_á$ line in these kinds of plasmas by up to (15 – 20)%.

Our third example relates to plasmas of radiofrequency discharges, such as, e.g., those studied in papers [28-30]. The plasma parameters, e.g., in the experiments [28, 29], are $N_e = 1.2\text{x}10^{13}$ cm^{-3} and $T = (1850 – 2000)$ K, i.e., $T = (0.16 – 0.17)$ eV. For the H_α line emitted from such a hydrogen plasma, the ratio from Eq. (60) yields 1.18 for C = 2 and 1.13 for C = 3/2. Figure 2 presents this ratio (for the H_α line emitted from a hydrogen plasma) versus the electron density N_e at T = 0.17 eV for $C = 2$ (solid line) and for $C = 3/2$ (dashed line). It is seen that the allowance for the CM motion increases the ion dynamical Stark width of the H_α line in these kinds of plasmas by up to (15 – 20)%.

4. CONCLUSIONS

We studied the general problem whether the CM motion and the relative motion can be separated for hydrogenic atoms/ions in a nonuniform electric field. We demonstrated that, strictly speaking, they cannot be separated. Then we used the approximate analytical method of the separation of rapid and slow subsystems to achieve the

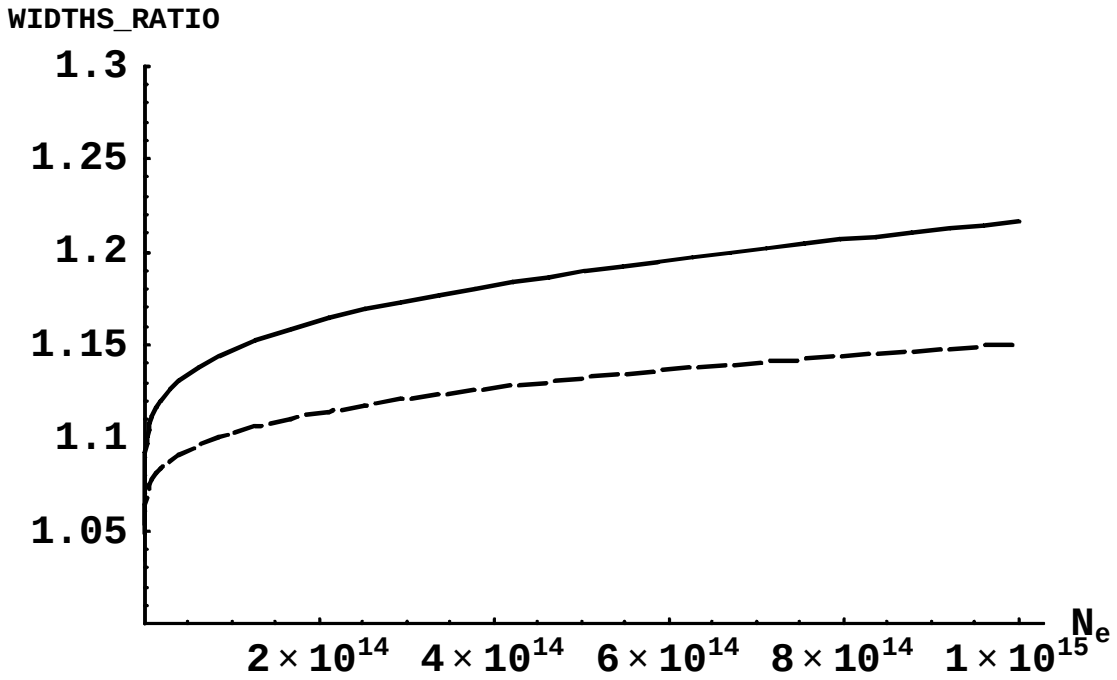

Figure 1: The ratio of the ion dynamical Stark width with the allowance for the center-of-mass motion to the ion dynamical Stark width from the conventional theory [20] versus the electron density N_e (cm^{-3}) for the $H_á$ line emitted from a hydrogen plasma at T = 1 eV for C = 2 (solid line) and for C = 3/2 (dashed line). Plasma parameters correspond to edge plasmas of magnetic fusion machines and to atmospheres of flare stars

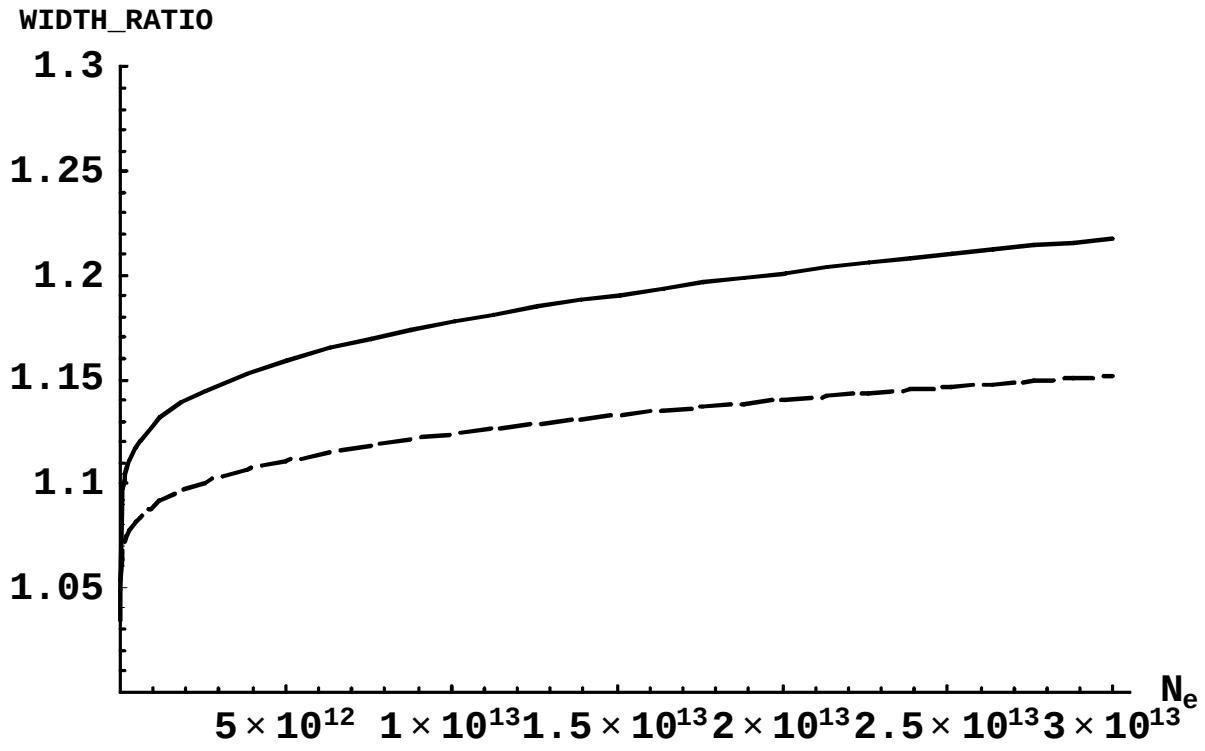

Figure 2: The ratio of the ion dynamical Stark width with the allowance for the center-of-mass motion to the ion dynamical Stark width from the conventional theory [20] versus the electron density N_e (cm^{-3}) for the H_α line emitted from a hydrogen plasma at T = 0.17 eV for C = 2 (solid line) and for C = 3/2 (dashed line). Plasma parameters correspond to radiofrequency discharges

pseudoseparation of the CM and relative motions for hydrogenic atoms/ion in an arbitrary nonuniform electric field. This is a fundamental result in its own right.

Next we further developed these results for the case of a hydrogen atom in the nonuniform electric field, where the field is due to the nearest (to the hydrogen atom) ion in a plasma. We showed that the effect of the CM motion can be formally taken into account via the substitution of the initial relative velocity V_0 in the pair "atom – ion" by an effective velocity V_{eff} that depends on the quantum numbers of the hydrogen atom, as well as on the initial separation R_0 in the pair "atom-ion" and on the ion charge Z.

Then we applied the results to the ion dynamical Stark broadening of hydrogen lines in plasmas. We obtained analytical results for the cross-sections of the optical collisions that control the corresponding Stark width. We presented specific examples of laboratory plasmas (such as magnetic fusion plasmas or plasmas of radiofrequency discharges) and astrophysical plasmas (such as in atmospheres of flare stars) where the allowance for these CM effects leads to a significant increase of the width of hydrogen spectral lines – by up to (15 – 20)%.

Thus, in addition to the fundamental importance, the results of the present paper seem to have also practical importance for spectroscopic diagnostics of laboratory and astrophysical plasmas.

Appendix A. Validity condition for the ion dynamical Stark broadening

The ion dynamical Stark broadening of hydrogen spectral lines is effective when the number ν_{Wi} of perturbing ions in the sphere of the ion Weisskopf radius is smaller than unity – see, e.g., review [7]. (In the opposite case of $\nu_{Wi} >> 1$, the perturbing ions can be treated in the quasistatic approximation.) By using the ion Weisskopf radius $R_{WA}(C)$ defined in Eq. (50), one arrives to the following validity condition:

$$\nu_{Wi}(C) = [3^{1/2}\pi/(2C^{3/2})](m_r/T)^{3/2}[(n^2 - n'^2)\hbar/\mu]^3 Z^2 N_e < 1. \quad (A.1)$$

For $C = 3/2$ (which is the choice of the strong collision constant in the conventional theory by Griem [20]) the numerical coefficient in the first brackets in the right side of Eq. (A.1) becomes $2^{1/2}\pi/3$. Thus, the ion dynamical Stark broadening can become effective for the most intense hydrogen spectral lines (i.e., for low values of n and n') in plasmas of relatively low electron densities.

Under the condition (A.1), for the overwhelming majority of perturbing ions, the frequency of the variation of the ion field v_i / R_N, where R_N is the mean interionic distance, exceeds the instantaneous Stark splitting in the ion field. Therefore the above requirement is called the modulation-type condition.

We note that there is another condition in Griem book [20], Eq. (82): $v_i / R_N > \gamma_e$, where γ_e is the electron impact width. This kind of requirement is called the damping-type condition. While both the modulation-type condition and the damping-type condition are necessary, the modulation-type condition (A.1) is more restrictive: it requires the electron (and ion) density to be by the factor $\sim (m_p/m_e)^{3/4} \sim 300$ smaller than the damping-type condition. Thus, the modulation-type condition overrides the damping-type condition.

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