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THEORETICALLY BASED CLOSED FORM FORMULAS FOR THE COLLISION OPERATOR FOR ISOLATED ION LINES IN THE STANDARD STARK-BROADENING THEORY

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Abstract—In this work we obtain closed form expressions for the collision operator for Stark broadening of isolated ion lines in the semiclassical (dipole) impact approximation and for a Maxwellian electron velocity distribution. These expressions are simple in that no integrations are involved, exact within the stated approximations, and apply equally to hot and cold plasmas as long as the above approximations are satisfied. These formulas give widths with good accuracy, together with an estimate of the theoretical error. Therefore, they can be used for fast data analysis and also for the calculation of a large number of lines, as, for example, in opacity calculations. In addition, the behavior of the collision operator as a function of the energy separation of the perturbing levels, the temperature, and the cutoffs becomes more transparent.

1. INTRODUCTION

For a number of applications, widths of isolated ion lines are required. Calculations of line broadening for such lines in a plasma are normally done using the impact approximation for electrons, in its semiclassical[1–3] or quantum-mechanical[4–6] version. For a wide range of plasma parameters, the semiclassical calculations, perhaps supplemented by a calculation of resonances, should be quite adequate and their theory is well-known.[7–10] Yet, partly because the relevant broadening (Coulomb excitation) functions are awkward to express in terms of elementary functions,[11] often semiempirical[11,12] or simplified semiclassical[13] formulas are used, which give closed form expressions. Agreement between the formulas and experiment is generally within a factor of 2. In the general case, it is possible, by using the Poquerusse expressions,[14] to reduce the relevant collision operator to an integral over velocity, to be evaluated at each of the energy separations of interest.[15] Other expressions[16] also reduce to integrals over velocity, but they are most valid for hydrogenic lines in hot plasmas.

The purpose of the present work is to give accurate, within the semiclassical dipole impact approximation, and easy to use (ideally as easy as the semiempirical formulas) *closed form* expressions for the linebroadening operator $\phi(\omega)$ as a function of the energy difference ω between the level in question and the perturbing level. These expressions are by no means "semiempirical" and are, within some very satisfactory numerical approximations to the relevant special functions, as exact, except for unitary considerations, as the semiclassical (dipole) impact approximation. Qualitatively, as illustrated in Fig. 1, this operator $\phi(\omega)$ starts off at the hydrogenic value at 0 energy spacing and *increases* for a while until it starts dropping.

The reason for this behavior (the "spike" in Fig. 1) is simply that the collision operator is the difference $f_- - f_+$ of the same function f, to be defined below, evaluated at the minimum and maximum impact parameters. For small ω, the contribution from the maximum impact parameter

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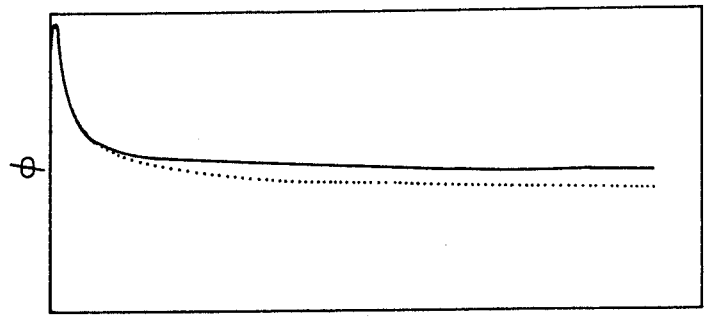

Fig. 1. Typical behavior of $\phi(\omega)$ vs ω. The solid line is for a vanishing ρ_- and the dotted line for a nonzero ρ_-, illustrating that for large ω, the choice of ρ_- is critical.

may be substantially reduced due to a part of the velocity phase space becoming adiabatic, while the contribution from the minimum impact parameter is still diabatic, hence their difference increases. In the limit of infinite energy separation, at which point the semiclassical approximation is not valid anyway, the collision operator has dropped to a constant value if the minimum impact parameter is allowed to be 0 or to 0 if it is not. The semiempirical[11,12] and simplified semiclassical[13] formulas give a decaying operator with increasing energy spacing and, failing to notice the "spike" at small energy spacings, they usually underestimate the weak collision contribution to the width. In contrast to semiempirical expressions the expressions derived here are "exact" in the sense that the only approximations involved are satisfactory fits of the relevant functions by simpler functions and the neglect of terms that will affect the result by 5–6% at the very most. Although including these terms is in principle no more difficult than some of the terms already included, we try to keep our formulas as simple as possible. Such expressions should be useful for experimentalists and also in cases where gains in speed without sacrificing accuracy are essential, e.g. opacity calculations. It should be noted that the expressions derived here are satisfactory as long as the semiclassical dipole impact approximation is satisfactory, and work equally well in hot and cold plasmas. They should be particularly useful as far as the temperature scaling is concerned. Contributions from higher multipoles, resonances, and ions, whether dynamic or quasistatic, are not considered in this work. It is possible to obtain error bounds for the linebroadening operator as, for example, in Ref. 15.

2. THEORY

Let

$$\xi = \omega\alpha v^{-3} \tag{1}$$

where v is the perturber velocity, ω is the energy separation between the level in question (upper or lower) and the perturbing level and

$$\alpha = \frac{(Z-1)e^2}{4\pi\epsilon_0 m} \tag{2}$$

with Z the spectroscopic charge number. The sign of ω does not matter and is taken here to be positive. We must emphasize that we are dealing with the impact and *not* the unified theory, so that ω does *not* refer to separation from the line center.

Let also

$$x = \xi^{-2/3} \tag{3}$$

and

$$q(\omega) = \frac{(\alpha\omega)^{2/3}m}{2kT}. \tag{4}$$

We also let ρ denote the impact parameter, i.e. the distance from the emitter to the asymptote of the hyperbolic trajectory. We use two such ρ, denoted ρ_+ and ρ_-, corresponding to the maximum and minimum impact parameters, respectively. Hereafter ρ and $\rho_\pm$ will be used interchangeably.

We also use

$$G(\omega) = \rho_\pm \left(\frac{\omega^2}{\alpha}\right)^{1/3} = \frac{2kT\rho \pm q(\omega)}{\alpha_m} \tag{5}$$

For simplicity of notation, we use q and G instead of $q(\omega)$ and $G(\omega)$.

We also define

$$\eta = Gx = \frac{\rho v^2}{\alpha} \tag{6}$$

in terms of which the eccentricity ϵ is

$$\epsilon = \sqrt{1 + \left(\frac{\rho v^2}{\alpha}\right)^2} = (1 + \eta^2)^{1/2} \tag{7}$$

and the adiabaticity parameter

$$\tau = \xi(\eta - \arctan \eta). \tag{8}$$

The real part of the "direct"[15] collision operator which is the only one of interest for isolated lines is then

$$\phi(\omega) = C(f_+ - f_-), \tag{9}$$

where

$$C = \frac{-2\pi n}{3}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 \sqrt{\frac{2}{\pi}}\left(\frac{m}{kT}\right)^{3/2}(\alpha\omega)^{2/3} = \frac{-4\pi nq}{3}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 \sqrt{\frac{2m}{\pi kT}} \tag{10}$$

with n the electron density and

$$f_\pm = \int_0^\infty dx e^{-qx} a(x^{-3/2}, \epsilon_\pm), \tag{11}$$

where $\epsilon_\pm$ is given by (7) with $\rho_\pm$ instead of ρ and

$$a(\xi, \epsilon) = \xi\epsilon e^{\pi\xi} |K_{i\xi}(\xi, \epsilon)| |K'_{i\xi}(\xi, \epsilon)|, \tag{12}$$

where

$$K_{i\xi}(\xi\epsilon) = \int_0^\infty du \cos \xi u e^{-\xi\epsilon \cosh u} \tag{13}$$

and

$$K'_{i\xi}(\xi\epsilon) = \int_0^\infty du \cos \xi u \cosh u e^{-\xi\epsilon \cosh u} \tag{14}$$

are the modified Bessel function of imaginary order $i\xi$ and its derivative respectively.

In terms of $\phi(\omega)$, the impact HWHM Φ is, therefore,

$$\Phi = \sum_{\alpha'} \phi(\omega_{\alpha\alpha'}) \frac{R^2_{\alpha\alpha'}}{2J_\alpha + 1} + \sum_{\beta'} \phi(\omega_{\beta\beta'}) \frac{R^2_{\beta\beta'}}{2J_\beta + 1}, \tag{15}$$

where α and β are the upper and lower levels respectively and α' and β' are their dipole-connected perturbing levels. R_{ij} is proportional to or equal to, depending on its definition, the reduced matrix element between i and j, so that R^2 may be obtained from the oscillator strengths f from

$$R^2 = \frac{3\hbar(2J_L + 1)f}{2m\omega},$$

with the subscript L referring to lower level, that is the lower of the α, α' and β, β' levels respectively.

The object of this work is to find analytic expressions for the integrals $f_\pm$ as a function of $\rho_\pm$ and ω. Thus, to calculate the width from Eqs. (9–15), one only needs to specify minimum and maximum impact parameters ρ_- and ρ_+. The choices for $\rho_\pm$ are discussed in the literature and our formulas apply for velocity-independent $\rho_\pm$. The maximum impact parameter ρ_+, of the order of the Debye length is indeed velocity-independent and, therefore, the only velocity dependence that we neglect here is in ρ_-. In the dipole approximation, it is often the case that the velocities for which unitarity is violated are too large and, therefore, have only negligible probability. In that case, taking $\rho_- = 0$ does not violate unitarity and in effect calculates the contribution of collisions that cannot be treated within the standard semiclassical impact approximation as if they were weak, semiclassical collisions. This is clearly only one out of many possible ways of estimating their contribution, which is unknown within the standard semiclassical approximation and only bounds may be obtained from unitarity considerations, e.g. Lorentz–Weisskopf. It is also possible to use a ρ_- different from 0, say the relevant wavefunction extent $(n_u^2 - n_l^2)a_0/Z$ with n_u and n_l the principal quantum numbers of the upper and lower levels, respectively, and a_0 the Bohr radius. Another possibility is to do a piecewise integration using a velocity-dependent cutoff as dictated by De Broglie and unitarity considerations, i.e. use a piecewise constant ρ_-. Evidently, the difficulty in using a velocity-dependent minimum impact parameter is that the integration is much harder to do in closed form and that ρ_- must be determined by solving Eq. (16) numerically, which would then speak for a fully numerical approach. The minimum impact parameter is the relevant wavefunction extent for $v \geqslant 2.18 \times 10^6 \frac{Z}{n_u^2}$ m/sec, with Z the spectroscopic charge and n_u the principal quantum number of the upper level if the unitarity cutoff is not important. As a final word of warning on these considerations, one should also note that $\rho_-(v)$ must in general be determined by solving the equation

$$\frac{2}{3}\left(\frac{mv}{\hbar Z_{em}\epsilon(\rho_-, v)}\right)^2 \left\{\sum_{\alpha'} \frac{R^2_{\alpha\alpha'}}{2J_\alpha + 1} A[\xi(v, \omega_{\alpha\alpha'}), \epsilon(\rho_-, v)] + \sum_{\beta'} \frac{R^2_{\beta\beta'}}{2J_\beta + 1} A[\xi(v, \omega_{\beta\beta'}), \epsilon(\rho_-, v)]\right\} = 1 \tag{16}$$

[another version of Eq. (16) is to have a RHS of 0.5 instead of 1] with the attractive A-function defined by:

$$A(\xi, \epsilon) = \xi^2 e^{\pi\xi}[|\epsilon K'_{i\xi}(\xi\epsilon)|^2 + (\epsilon^2 - 1)|K_{i\xi}(\xi\epsilon)|^2]. \tag{17}$$

The function $A(\xi, \epsilon)$ is thus essential for the determination of the minimum impact parameter. Such a determination is especially important for ion impact calculations, which are, however, usually unimportant for nonhydrogenic ions, at least in the dipole approximation considered here. A is harder to approximate than a, because of its behavior very close to $\epsilon = 1$. Nevertheless, closed-form analytical formulas are possible.[17] Since we want to give a closed formula for the width, we necessarily neglect considerations involved in a fully consistent determination of the minimum impact parameter $\rho_-(v)$. One can check the final result against unitarity considerations.

The function $a(\xi, \epsilon)$ is given by Poquerusse's analytical fits: if $\tau \geqslant 0.15$

$$a(\xi, \epsilon) = e^{-2\tau}\left(1.5723 + \frac{0.35996}{\tau} - \frac{0.4501}{\epsilon\tau} - \frac{0.0686}{\tau^2} + \frac{0.12495}{\epsilon^2\tau} + \frac{0.10219}{\epsilon\tau^2} + \frac{0.009291}{\tau^3} - \frac{0.03921}{\epsilon^2\tau^2} - \frac{0.011913}{\epsilon\tau^3} - \frac{5.1127}{(10\tau)^4} + \frac{2.9632}{(10\tau)^3\epsilon^2} + \frac{5.17}{(10\tau)^4\epsilon}\right). \tag{18}$$

For simplicity we refer to this regime as "adiabatic".

If $\tau \leqslant 0.15$ and $\xi \leqslant 0.2$ we are in the "hydrogenic" regime

$$a(\xi, \epsilon) = L + 3.143\xi L - \xi^2 L(1.47 + 0.446\epsilon^2 L + 0.501L^2) + 6.52\xi^2 - 10.54\xi^3 - 12.4\xi\tau^2 + 54\xi\tau^3 \tag{19}$$

with

$$L = -\gamma + \ln(2/\xi\epsilon) = \ln 2 - \gamma - \ln(\xi\epsilon) = 0.116003675 - \ln(\xi\epsilon) \tag{20}$$

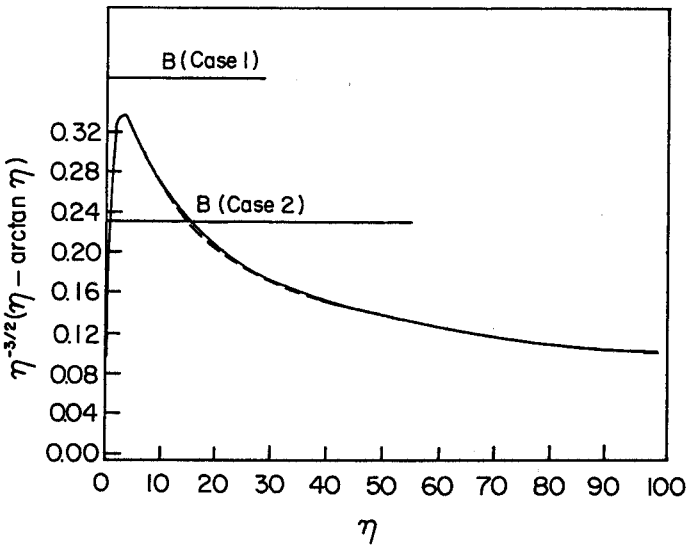

Fig. 2. The exact function $\eta^{-3/2}(\eta - \arctan\eta)$ is the solid line and the dashed line is the approximation given by Eq. (25). The horizontal straight lines are values of B defined by Eq. (22). For the highest B there is no intersection and no adiabatic contribution (Case 1), while for the lower B the region between the two points of intersection is adiabatic (Case 2).

and γ the Euler constant ($=0.577215\ldots$), while if $0.2 \leqslant \xi$ and $\tau \leqslant 0.15$ we have

$$a(\xi,\epsilon) = \frac{\pi}{\sqrt{3}} + 0.40215\xi^{-2/3} - 1.7252\tau^{2/3} - 0.0364\xi^{-4/3} + 0.00203\xi^{-2}$$
$$- 0.86123\xi^{-2/3}\tau^{2/3} - 1.941\tau^{4/3} + 0.6744\xi^{-2/3}\tau^{4/3} + 2.834\tau^2 + 0.04023\xi^{-4/3}\tau^{4/3}. \quad (21)$$

For lack of a better name, we refer to this regime as "inelastic". The last two terms of $a(\xi,\epsilon)$ are less than 3.5% and 1.5% of the first term in Eq. (21) and can be safely neglected.

The Poquerusse expressions are excellent approximations to the a-function and it can be shown[17] that they give the correct asymptotic behavior.

Defining

$$B = \frac{0.15}{\omega}\sqrt{\frac{\alpha}{\rho_{\pm}^3}} = 0.15G^{-3/2} \quad (22)$$

the equation $\tau = 0.15$ reads

$$\eta^{-3/2}(\eta - \arctan\eta) = B \quad (23)$$

When we graphically solve this equation, as shown in Fig. 2, we find that we have no solution for $B > 0.3375488$, in which case $\tau \leqslant 0.15$. In terms of ω, $\tau \leqslant 0.15$ for

$$\omega \leqslant 0.444380185\sqrt{\frac{\alpha}{\rho_{\pm}^3}}. \quad (24)$$

We refer to this case as Case 1. In this regime, the collision operator as defined by Eq. (9) is least dependent on the choice of the minimum impact parameter and, hence, most certain and the semiclassical approach is at its best. In contrast, in the large energy separation regime, relatively small variations in the minimum impact parameter produce large variations in the collision operator. Of course, for $\rho_- = 0$, τ is always less than 0.15.

For $B < 0.3375488$, called here Case 2, there are two solutions. The region between these two solutions corresponds to adiabatic collisions, i.e. $a(\xi,\epsilon)$ is given by Eq. (18). This is also to be expected on physical grounds, as for ion lines, adiabaticity is an *intermediate* and not a small velocity effect.

It is now essential to obtain expressions for $\tau(x)$ that can be integrated analytically and also to solve the equation $\tau = 0.15$, or, equivalently, Eq. (23).

From a simple asymptotic analysis, we can derive the following approximation

$$\eta^{-3/2}(\eta - \arctan\eta) \approx \frac{\eta^{3/2}}{3 + 0.8\eta + 0.2\eta^{3/2} + \eta^2} \tag{25}$$

which is shown as the dashed line in Fig. 2. Then Eq. (23) is a quartic equation in $z = \eta^{1/2}$ and its solution is known in closed form.

It is possible, and in some cases advantageous, to have a similar formula for $\tau^{2/3}$. Now

$$\tau = G^{3/2}\eta^{-3/2}(\eta - \arctan\eta) \tag{26}$$

and

$$\tau^{2/3} = G\eta^{-1}(\eta - \arctan\eta)^{2/3} \tag{27}$$

Again, from asymptotic considerations we can obtain the following approximation for $\tau^{2/3}$

$$\tau^{2/3} = G\frac{\eta}{3^{2/3} + \eta^{4/3}} \tag{28}$$

This is an alternative to Eq. (25) as far as solving for $\tau = 0.15$, since it leads to a simpler quartic equation, but is still not too useful for performing the integrals analytically. There is, of course, no problem in solving $\tau = 0.15$ numerically for Case 2; nevertheless, with say Eq. (28) this can be done analytically also, although some care is required for $0.58233 \leqslant G \leqslant 0.59493$.

Having established the existence of two cases, we will write the quantity $f_\pm$ for each case in terms of only two functions, $W_1(x, q, G)$ and $W_2(x, q, G)$, which are "universal" in the sense that they are needed for both cases and only their x argument changes. These functions are given in Appendix A, with some derivations presented in Appendix B and approximations for some required special functions given in Appendix C.

3. $f_\pm$ FOR CASE 1

Since $\tau \leqslant 0.15$ in this case, there are two regions in the integration: $x \leqslant 0.2^{-2/3} = x_0 = 2.924017738$ ($\xi \geqslant 0.2$) and $x \geqslant x_0$ ($\xi \leqslant 0.2$) Accordingly we obtain

$$f_\pm = W_1(x_0, q, G) + W_2(x_0, q, G). \tag{29}$$

Equation (29), which is valid for $\omega \leqslant 0.444380185\sqrt{\frac{q}{\rho_\pm^3}}$, along with Eq. (9) is sufficient to determine the contribution of a dipole connected perturbing level at a frequency separation ω to $\phi(\omega)$.

4. $f_\pm$ FOR CASE 2

Let us denote by η_1 and $\eta_2 > \eta_1$ the two solutions of Eq. (23) and define $x_1 = \eta_1/G$ and $x_2 = \eta_2/G$. The new feature is the adiabatic contribution from $x_1 \leqslant x \leqslant x_2$. Note that for Case 2, $Gx_0 \geqslant 1.7$. According to the position of $x_0 = 0.2^{-2/3}$, which discriminates between hydrogenic and inelastic collisions, we have two subcases, as shown in Fig. 3:

(a) $x_0 < x_1$. This happens if $Gx_0 < 1.81788$ (this number is the solution of y-arctan $y = 0.75$). Qualitatively, we have the inelastic region $(0, x_0)$, the hydrogenic regions (x_0, x_1) and (x_2, ∞), and the adiabatic region (x_1, x_2). Quantitatively, if the contribution of the adiabatic region is neglected, we may write $f_\pm$ for this subcase as

$$f_\pm = W_2(x_0, q, G) + W_1(x_0, q, G) - W_1(x_1, q, G) + W_1(x_2, q, G). \tag{30}$$

If the adiabatic contribution is not neglected, an adiabatic integral between x_1 and x_2 should be added. This is true for both subcases.

(b) $x_1 < x_0 < x_2$. This happens if $Gx_0 \geqslant 1.81788$. In this case we have the inelastic region $(0, x_1)$, the adiabatic region (x_1, x_2), and the hydrogenic (x_2, ∞). Again, neglecting the adiabatic contribution we have

$$f_\pm = W_1(x_2, q, G) + W_2(x_1, q, G). \tag{31}$$

We can also give a simple expression for x_1 based on (A16):

$$x_1 = \frac{1}{2G}\left[\frac{15}{4} - \left[\left(\frac{15}{4}\right)^2 - 15(3B)^{2/3}\right]^{1/2}\right] \tag{32}$$

It can be easily shown, both analytically and graphically, that there can be no case where the inelastic region is interrupted by the adiabatic region.

The contribution of the adiabatic region (x_1, x_2), is expected to be small due to the damping factors $e^{-2\tau}$ in Eq. (18): Although for $\tau \approx 0.15$, the adiabatic a-function is still appreciable, it drops fast with increasing τ, so that it may be reasonable to neglect its contribution to the $f_\pm$ integrals. Nevertheless, it may happen that the adiabatic region is so large that it covers virtually all of the region where the Maxwell–Boltzmann distribution is appreciable, so that the adiabatic contribution is comparable to or larger than the sum of the hydrogenic and inelastic contributions. In such a case, one should probably include quadrupole terms, for which the "hydrogenic" channel $\omega = 0$ is always available. In addition, other mechanisms, such as Doppler broadening are probably more important than Stark broadening.

5. CONCLUSIONS AND A WORD OF WARNING

We have given *closed form* expressions for the electron dipole impact collision operator and, hence, the width as a function of the energy difference between the upper or lower level and the perturbing level for isolated ion lines. The actual width (FWHM) should be between this width and this width plus

$$4\pi n \rho_-^2 \left(\frac{2kT}{\pi m}\right)^{1/2} \{1 - S_a S_b\}$$

with the factor $\{1 - S_a S_b\}$ between 0 and 2. This extra term is the strong collision contribution, assuming a constant ρ_-, i.e., that de Broglie and unitarity considerations are unimportant. For high densities or low temperatures it may be comparable to or even larger than the weak contribution, indicating that the standard semiclassical impact approximation is unsatisfactory and a more precise calculation of the strong collision term is required.

Although less simple than the semiempirical formulas, these formulas are *closed form* and, furthermore, there are simplifications in these formulas if one takes, for example, the minimum impact parameter to be 0. We used some numerical approximations, which are quite satisfactory, by comparison to the accuracy obtained in semiclassical calculations. Within these numerical approximations, our formulas are as good as an exact semiclassical dipole impact calculation,

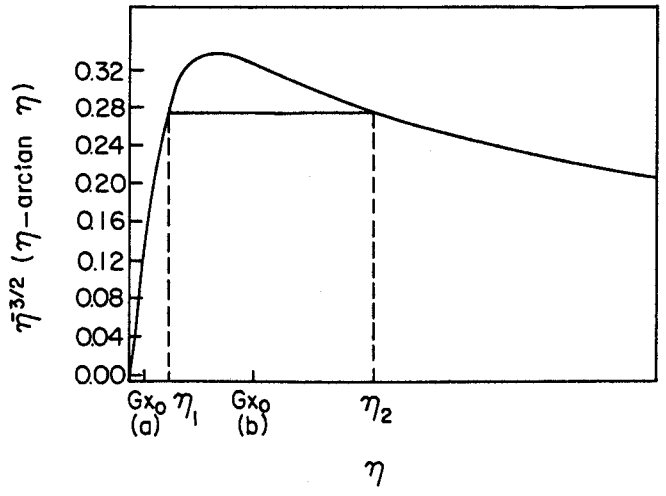

Fig. 3. The function $\eta^{-3/2}(\eta - \arctan\eta)$ for Case 2 for a value of B that is given by the horizontal line segment. Also shown are two possible values of Gx_0. The smaller one corresponds to subcase *a* and the larger one to subcase *b*.

provided that unitarity is not violated for all velocities with appreciable probability density. This will be the case if one can find a minimum impact parameter, for example the relevant wavefunction extent, such that unitarity is satisfied for all velocities with appreciable probability density, without considerably increasing the strong collision phase space. Also, because our formulas are theoretically based, they may be expected to perform well even in regimes where there are no experimental data, provided the underlying assumptions hold. In addition, they provide insight into the actual behavior of the collision operator, for example the hydrogenic, inelastic and adiabatic contributions. In particular, the dependence of the collision operator and, thus, the line width on energy separation, minimum and maximum impact parameters, and temperature is rather complex, but is nevertheless given in closed form. These formulas give a prediction for the Stark width scaling with temperature, which has not been sufficiently studied[18] as yet. It appears that experimental work may shed light in this area.[18-20]

Recent precision experiments [20,21] for the $3p - 3s$ Li-like lines suggest that at least for the conditions of these experiments, the above formulas may be more accurate than the commonly used semiempirical[11,12] or simplified semiclassical[13] formulas. Nevertheless, more comparisons are needed to reach definite conclusions as to the accuracy of the present formulas. We note, however, that the present formulas, if in poor agreement with experiment, point out to some effects to be examined, e.g., unitarity considerations, strong collision terms, adiabatic contributions and sources that are outside the scope of this work, i.e., higher multipoles, ionic contributions, resonances (all of which are usually treated as additive contributions to the width), and Doppler and natural broadening.

The most important approximation in this work is the neglect of unitarity considerations that may necessitate a velocity-dependent minimum impact parameter. Failure to account for this, as in the formulas given, could result in overestimating the collision operator and hence the width.[22] One should recall, however, that also semiempirical[11,12] and simplified semiclassical[13] formulas can only treat unitarity roughly, using a hydrogenic cutoff for example,[13] which has been shown in Ref. 15 to underestimate ρ_- by a factor as large as 5. Since, unlike a self-consistent calculation, as for example in Ref. 15, these formulas cannot deal with unitarity considerations, they cannot be extended to include quadrupole interactions. In addition, the usual problems of the standard semiclassical approximation apply.[3,11] For example, for large energy separations the choice of the minimum impact parameter is critical.

In summary, we have given new closed form expressions, which, together with the strong collision error bars, may be used for fast and accurate calculations of Stark widths of isolated ion lines and also of the diagonal part of the partially overlapping collision operator. If the error bars are too large due to quantum effects, one should resort to other methods,[6] while if these widths prove to be inaccurate due to unitarity violation, a fully numerical calculation[8,15] should, strictly speaking, be done. In the framework of the present work, one may, as the implementation[22] of these formulas can do, use a (larger) constant ρ_-, equal to the exact ρ_- at the average velocity. This enables one to use the present formulas, while minimizing the severity of unitarity violation.

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APPENDIX A

The W_1 and W_2 Functions

We define the hydrogenic contribution

$$W_1(x_0, q, G) = H_1 + H_2 + H_6 + H_7 \tag{A1}$$

where in H_i the subscript refers to the hydrogenic term in Eq. (19) that produces the stated contribution. Note that five out of the total nine terms are neglected for reasons explained in Appendix B. Thus, H_1 is given by

$$H_1 = \int_{x_0}^{\infty} dx e^{-qx} L = \frac{e^{-qx_0}}{q}(1.5 \ln x_0 + s) + 1.5\frac{E_1(qx_0)}{q} - \frac{1}{2G}P_1(\lambda, Gx_0) \tag{A2}$$

where

$$s = \ln 2 - \gamma = 0.11600368 \tag{A3}$$

λ is defined as

$$\lambda = \frac{q}{G} = \frac{\alpha m}{2kT\rho_{\pm}} = \frac{7.2178(Z-1)}{T(\text{eV})\rho_{\pm}(\text{Å})} \tag{A4}$$

where $T(\text{eV})$ and $\rho_{\pm}(\text{Å})$ mean that T is in eV and the impact parameter is in Å, $E_n(x)$ is the exponential integral

$$E_n(x) = \int_1^{\infty} dt \frac{e^{-xt}}{t^n} = x^{n-1}\int_x^{\infty} dt \frac{e^{-t}}{t^n} = x^{n-1}\Gamma(1-n, x) \tag{A5}$$

and

$$P_1(\lambda, x) = \int_x^{\infty} e^{-\lambda y} \ln(1+y^2) dy. \tag{A6}$$

Similarly, H_2 is

$$H_2 = 3.143\int_{x_0}^{\infty} dx e^{-qx} L x^{-3/2}$$

$$= 1.5715\left[2sq^{1/2}\Gamma\left(-\frac{1}{2}, qx_0\right) - G^{1/2}P_2(\lambda, Gx_0) + \frac{6S_1(qx_0, x_0)}{x_0^{1/2}}\right] \tag{A7}$$

where

$$P_2(\lambda, x) = \int_x^{\infty} dy e^{-\lambda y}\frac{\ln(1+y^2)}{y^{3/2}} \tag{A8}$$

and

$$S_1(y, x) = (2 + \ln x)\left[e^{-y} - y^{1/2}\Gamma\left(\frac{1}{2}, y\right)\right] - \sqrt{y}\int_y^{\infty}\frac{dt e^{-t}}{t^{1/2}}\ln\frac{t}{y} \tag{A9}$$

with $\Gamma(a, x)$ denoting an incomplete Gamma-function

$$\Gamma(a, x) = \int_x^\infty dt e^{-t} t^{a-1}. \tag{A10}$$

Evidently, incomplete Gamma functions with a half-integer a may be expressed in terms of $\Gamma(\frac{1}{2}, x)$, but we have not done so in order to keep these formulas more compact. Finally

$$H_6 = \int_{x_0}^\infty dx e^{-qx} 6.52 x^{-3} = 3.26\left[\frac{e^{-qx_0}(1 - qx_0)}{x_0^2} + q^2 E_1(qx_0)\right] \tag{A11}$$

and

$$H_7 = -\int_{x_0}^\infty dx e^{-qx} 10.54 x^{-9/2} = -10.54 q^{7/2}\Gamma\left(-\frac{7}{2}, qx_0\right). \tag{A12}$$

It may be shown that only the term involving P_1 remains in the limit $\omega \to 0$ in Eq. (9), since, as said above, the other terms in H_1 from f_- and f_+ cancell. This is, evidently, the well-known hydrogenic limit[3] involving the integral over velocities of $\ln \frac{\zeta_+}{\zeta_-}$. This is the only remaining term for $\omega \leqslant 0.444380185\sqrt{\frac{\pi}{\rho_+^3}}$, since $\rho_\pm$ does not appear in the remaining terms and hence the maximum and minimum impact parameter contributions cancel. This is important for the numerical implementation because the total contribution (i.e., multiplied by C) from H_1 diverges as $q \to 0$ due to the exponential integral term.

In Appendix C we construct analytic approximations for S_1, P_1, and P_2. For the inelastic contribution

$$W_2(x, q, G) = I_1(x, q) + I_2(x, q, G) \tag{A13}$$

where I_1 is the term obtained by integrating the terms in the inelastic contribution that do *not* involve τ

$$I_1(x, q) = \frac{(1 - e^{-qx})\pi}{q\sqrt{3}} + \frac{0.40215[1 - (1 + qx)e^{-qx}]}{q^2}$$
$$- \frac{0.0364[2 - 2e^{-qx}(1 + qx) - e^{-qx}q^2x^2]}{q^3} + 0.00203\frac{[6 - 6(1 + qx)e^{-qx} - e^{-qx}(3q^2x^2 + q^3x^3)]}{q^4}. \tag{A14}$$

Note that I_1 is well-behaved as $q \to 0$.

As for the terms involving τ, we need the integral

$$I_2(x, q, G) = \int_0^x dx e^{-qx}\tau^{2/3}(-1.7252 - 0.86213x - 1.941\tau^{2/3} + 0.6744x\tau^{2/3}) \tag{A15}$$

where, as already discussed, we have dropped the last two terms in Eq. (21). We note that these two terms could be integrated as the other terms, using the approximation to be discussed below. However, we neglect them since they do not add to the accuracy of these calculations.

In Case 1 we see that with the bound on ω, $\eta \leqslant 1.7$. Thus we need an approximation to $\tau^{2/3}$ for $\eta \leqslant 1.7$. The polynomial approximation

$$\tau^{2/3} = 3^{-2/3}G^2 x\left(1 - \frac{4}{15}Gx\right) \tag{A16}$$

gives better than 5% accuracy over the entire region of interest and an integral that can be done in closed form. For Case 2, the maximum η is 1.81788 [the solution of $\tau(\xi = 0.2) = 0.15$] and the above approximation is still better than 5%. Consequently, we obtain

$$I_2(x, q, G) =$$
$$0.829389653G^2N_1 - (0.414468874 - 0.221170574G + 0.448604744G^2)G^2N_2$$
$$+ (0.110525032 + 0.155867614G + 0.239255863G^2)G^3N_3$$
$$- (0.083129394 + 0.031900781G)G^5N_4 + 0.011083919G^6N_5 \tag{A17}$$

with

$$N_k = \int_0^x \mathrm{d}x \mathrm{e}^{-qx} x^k \tag{A18}$$

i.e.

$$N_1 = \frac{1 - \mathrm{e}^{-qx} - \mathrm{e}^{-qx} qx}{q^2} \tag{A19}$$

$$N_2 = \frac{2(1 - \mathrm{e}^{-qx}) - \mathrm{e}^{-qx}[(qx)^2 + 2qx]}{q^3} \tag{A20}$$

$$N_3 = \frac{6(1 - \mathrm{e}^{-qx}) - \mathrm{e}^{-qx}[(qx)^3 + 3(qx)^2 + 6qx]}{q^4} \tag{A21}$$

$$N_4 = \frac{24(1 - \mathrm{e}^{-qx}) - \mathrm{e}^{-qx}[(qx)^4 + 4(qx)^3 + 12(qx)^2 + 24qx]}{q^5} \tag{A22}$$

$$N_5 = \frac{120(1 - \mathrm{e}^{-qx}) - \mathrm{e}^{-qx}[(qx)^5 + 5(qx)^4 + 20(qx)^3 + 60(qx)^2 + 120qx]}{q^6}. \tag{A23}$$

Some care is needed in the numerical implementation for small q.

APPENDIX B

Derivation of the Formulas

In this Appendix we justify our approximation for the hydrogenic case integral. We consider the hydrogenic contribution from some x_i to ∞. In Case 1, $x_i = 0.2^{-2/3}$. In Case 2, $x_i \geqslant 0.2^{-2/3}$ since ξ must be $\leqslant 0.2$.

Specifically, we must justify neglecting the terms $-1.47L\xi^2$, $-0.446(\epsilon\xi L)^2$, $-0.0501L^3\xi^2$, $-12.4\xi\tau^2$ and $54\xi\tau^3$.

Starting with the first term, $1.47\xi^2 \leqslant 0.0588$ and thus this term is neglected compared to the first term (see H_1).

To estimate the next two terms, we have solved $\tau \leqslant 0.15$ and found the maximum ϵ for $\xi \leqslant 0.2$ (Fig. 4).

Thus $\epsilon\xi \leqslant 0.41$. The quantity $0.446\epsilon^2\xi^2 L$ is an increasing function of $\epsilon\xi$ with a maximum of about 0.075, hence this term can be neglected compared to the first term. Similarly, $0.501L^2\xi^2 \leqslant 0.501L^2\xi^2\epsilon^2$, and this is also an increasing function with a maximum of about 0.0854. Since at the maximum $\epsilon \approx 2.5$, this term is entirely negligible.

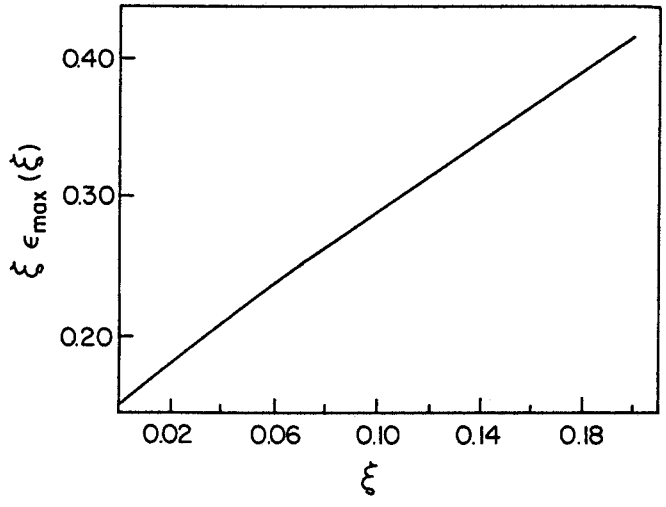

Fig. 4. $\xi\epsilon_{\max}(\xi)$ vs ξ with $\epsilon_{\max}(\xi)$ obtained from a numerical solution of the equation $\tau = 0.15$.

As for the last two terms

$$54x^{-3/2}\tau^3 \leqslant 0.0365 \tag{B1}$$

and

$$12.4x^{-3/2}\tau^2 \leqslant 0.0558. \tag{B2}$$

These terms are small compared to L, since $\ln(\epsilon\xi) \leqslant -0.9$ and thus $L \geqslant 1.016$. In addition

$$\int_{x_i}^{\infty} dx e^{-qx}(12.4x^{-3/2}\tau^2) \leqslant 0.0558 \frac{e^{-qx_i}}{q} \tag{B3}$$

and

$$\int_{x_i}^{\infty} dx e^{-qx}(54x^{-3/2}\tau^3) \leqslant 0.0364 \frac{e^{-qx_i}}{q} \tag{B4}$$

and both these terms for case 1 are negligible compared to the term from the inelastic contribution

$$\frac{-2.72802807e^{-qx_j}}{q}.$$

One should keep in mind that the x_j in the above expression is smaller than or equal to the x_i that appears in the hydrogenic contribution.

Since the net quantity of interest is the difference $f_- - f_+$, the question may be raised whether the neglected terms could play a role, should there be some cancellation in H_1 from the minimum and maximum impact parameters. However, this cancellation is most serious for small ω and the neglected terms are all higher order in ω than H_1.

APPENDIX C

Approximations for P_1, P_2, and S_1-functions

For $S_1(y, x)$, one needs to approximate the integral in (A9). The proposed approximation for

$$S_1'(y) = S_1(y, x) - (\ln x + 2)\left[e^{-y} - y^{1/2}\Gamma\left(\frac{1}{2}, y\right)\right] \tag{C1}$$

based on approximations to the integral in (A9) from small argument expansions, asymptotic expansions and Chebyshev fits is

$$\begin{aligned} S_1'(y) &= \sqrt{\pi y}\,[\ln y + \sqrt{\pi}\,(\gamma + 2\ln 2)] - 4y + \frac{4y^2}{9}, \quad y \leqslant 0.34 \\ &= \frac{e^{-y}}{y}\left(1 - \frac{2}{y} + \frac{23}{4y^2} - \frac{22}{y^3}\right), \quad y \geqslant 7 \\ &= \sqrt{y}\exp(-6.768870397 - 3.545845204z_1 + 0.2231008652z_1^2 - 0.157521305z_1^3 \\ &\quad + 0.0311681z_1^4 + 0.03204829957z_1^5 + 0.01843926253z_1^6), \quad 1.5 \leqslant y \leqslant 7 \\ &= \sqrt{y}\exp(-1.783373183 - 1.163688436z_2 + 0.142885452z_2^2 - 0.04717774z_2^3 \\ &\quad + 0.01851471z_2^4 - 0.017450451z_2^5 + 0.00973931039z_2^6), \quad 0.34 \leqslant y \leqslant 1.5 \end{aligned} \tag{C2}$$

where

$$z_1 = 0.3636363636y - 1.545454545 \tag{C3}$$

and

$$z_2 = 1.724137931y - 1.586206897. \tag{C4}$$

The accuracy of this approximation is better than 3.1% in all cases and usually much better than 3.1%. As a final remark on $S_1(y, x)$, this function is also used in the calculation of P_2. Note that x is always larger than $0.2^{-2/3} \approx 2.92$ in (A7), whether we are dealing with Case 1 or 2, and S_1 will

be needed in the calculation of P_2 for $x \geqslant 1.5$. Because of this lower bound on x, one can verify that

$$\frac{(2+\ln x)[e^{-y} - y^{1/2}\Gamma(\frac{1}{2}, y)]}{S_1'(y)} \geqslant 1 + \frac{\ln 1.5}{2} \approx 1.202. \tag{C5}$$

Consequently, the maximum relative error in S_1 due to cancellation between S_1' and $(2+\ln x)[e^{-y} - y^{1/2}\Gamma(\frac{1}{2}, y)]$ is about 9%.

For $P_1(\lambda, x)$, the limiting case of $x = 0$ is obtainable in closed form

$$P_1(\lambda, 0) = -\frac{2}{\lambda}[\cos\lambda \mathrm{ci}(\lambda) + \sin\lambda \mathrm{si}(\lambda)], \tag{C6}$$

where ci and si are the cosine and sine integrals respectively.

After a partial interation one obtains

$$P_1(\lambda, x) = \frac{e^{-\lambda x}}{\lambda}\ln(1+x^2) + \frac{2}{\lambda}\int_x^\infty \frac{y\,dy\,e^{-\lambda y}}{1+y^2}. \tag{C7}$$

The RHS integral is easily seen to reduce to $E_1(\lambda x)$ for large x and this approximation should be better the smaller the λ, since larger ys, for which the unity in the denominator may be neglected, make a larger contribution. It turns out that this approximation is numerically good for $x \geqslant 1.5$ for all λ. For small x ($x \leqslant 1$), one may do the integral analytically by expanding the logarithm or the exponential as a power series, i.e.

$$P_1(\lambda, x) = P_1(\lambda, 0) - \int_0^x dy\, e^{-\lambda y}\ln(1+y^2) \tag{C8}$$

and substitute the approximation given by Hastings:[23]

$$\ln(1+y^2) = b_1 y^2 + b_2 y^4 + b_3 y^6 + b_4 y^8, \quad y \leqslant 1 \tag{C9}$$

with $b_1 = 0.9974442$, $b_2 = -0.4712839$, $b_3 = 0.2256685$, $b_4 = -0.0587527$. This approximation is good to within 10% for $y \leqslant 1.4$ and to within 20% for $y \leqslant 1.5$. Of course, the relative error to P_1 will be smaller. With Eq. (C9), the RHS integral in Eq. (C8) may be evaluated in closed form. However, for small λ numerical problems arise. In that case, $P_1(\lambda, 0)$ dominates in Eq. (C8). Nevertheless, we can also keep the integral in Eq. (C8) by using the approximation $e^{-\lambda x} = 1$ for, say $\lambda < 0.1$, in which case we get

$$P_1(\lambda, x) = P_1(\lambda, 0) - [x\ln(1+x^2) + 2\arctan(x) - 2x]. \tag{C10}$$

The only problem with Eq. (C8) is that for large λ we are subtracting two nearly equal quantities and may expect serious cancellation. In that case, we can use the asymptotic expansion

$$P_1(\lambda, x) \approx \frac{e^{-\lambda x}}{\lambda}\left[\ln(1+x^2) + \frac{2x}{(1+x^2)\lambda} + \frac{2(1-x^2)}{\lambda^2(1+x^2)^2} + \cdots\right]. \tag{C11}$$

Thus, the recommended analytical representation of P_1 is: For $\lambda \leqslant 0.1$ and $x \leqslant 1.45$, P_1 is given by (C10). If $x \geqslant 1.45$

$$P_1(\lambda, x) = \frac{2E_1(\lambda x) + e^{-\lambda x}\ln(1+x^2)}{\lambda} \tag{C12}$$

and otherwise

$$\begin{aligned} P_1(\lambda, x) = P_1(\lambda, 0) - \Bigg\{ & \frac{1-e^{-\lambda x}}{\lambda^3}\left(\frac{40320b_4}{\lambda^6} + \frac{720b_3}{\lambda^4} + \frac{24b_2}{\lambda^2} + 2b_1\right) \\ & - e^{-\lambda x}\Bigg[\frac{x^2}{\lambda}(b_1 + b_2x^2 + b_3x^4 + b_4x^6) + \frac{x}{\lambda^2}(2b_1 + 4b_2x^2 + 6b_3x^4 + 8b_4x^6) \\ & + \frac{2x^2}{\lambda^3}(6b_2 + 15b_3x^2 + 28b_4x^4) + \frac{24x}{\lambda^4}(b_2 + 5b_3x^2 + 14b_4x^4) \\ & + \frac{x^2}{\lambda^5}(360b_3 + 1680b_4x^2) + \frac{x}{\lambda^6}(720b_3 + 6720b_4x^2) + \frac{20160b_4x}{\lambda^7}\left(x + \frac{2}{\lambda}\right)\Bigg]\Bigg\} \end{aligned} \tag{C13}$$

if $\lambda \leqslant Q_1(x)$ and Eq. (C11) if $\lambda > Q_1(x)$, where $Q_1(x)$ specifies beyond what λ one should use Eq. (C11) rather than Eq. (C13). A compromise between simplicity and accuracy is the approximation

$$\begin{aligned} Q_1(x) &= 15, x \leqslant 0.2 \\ &= 16 + 2.5833333x - 43.75x^2 + 29.16666667x^3, \quad 0.2 < x \leqslant 1 \\ &= -6 + 22.5x - 12.5x^2, \quad 1 < x \leqslant 1.4 \\ &= 1, \quad 1.4 < x \leqslant 1.45. \end{aligned} \tag{C14}$$

The proposed approximation for $P_1(\lambda, x)$ gives a maximum error of 10% (for $x \geqslant 1.45$ and $\lambda \leqslant 1$). Usually, the error is much less.

It may be seen that P_1 diverges as $\lambda \to 0$. When one considers the contribution to $\phi(\omega)$, i.e., when one accounts for an extra factor of λ arising from a q from C and the $1/G$ in (A2), one gets only a logarithmic divergence as $\lambda \to 0$. There are two ways that $\lambda \to 0$ can occur: either $T \to \infty$, in which case the contribution is 0 due to the remaining $T^{-1/2}$ factor in C, or $\rho \pm \to \infty$, which is expected, since we are using an unshielded interaction and are accounting for shielding via Debye cutoffs, so we cannot allow $\rho_\pm$ to get arbitrarily large.

The approximation of P_2 is obtained similarly. For $x \gg 1$, in practice $x \geqslant 1.5$ is adequate, we approximate $\ln(1+y^2) \approx 2 \ln y$ and with an integration by parts we obtain the approximation

$$P_2(\lambda, x) \approx \frac{4S_1(\lambda x, x)}{\sqrt{x}}. \tag{C15}$$

Approximation (C15) will be most inaccurate when $x = 1.5$ *and* $\lambda \to \infty$, so that the contribution to P_2 comes from a region very close to 1.5. In that case, the maximum error in approximating $\ln(1+y^2)$ by $2 \ln y$ (that is, at $y = 1.5$) is 30% and (C15) gives the same relative error. For P_1, on the other hand, the leading asymptotic contribution was given correctly in Eq. (C7) and this problem did not arise. To improve this situation, we will use the asymptotic expansion

$$P_2(\lambda, x) \approx \frac{e^{-\lambda x}}{\lambda x^{3/2}} \left[\ln(1+x^2) + \frac{\dfrac{2x^2}{1+x^2} - \dfrac{3}{2}\ln(1+x^2)}{\lambda x} + \frac{\dfrac{15}{4}\ln(1+x^2) - 4\dfrac{x^2(1+2x^2)}{(1+x^2)^2}}{\lambda^2 x^2} \right]. \tag{C16}$$

Thus, if one uses Eq. (C16) for $\lambda \geqslant 1$ and Eq. (C15) for $\lambda < 1$, one obtains $P_2(\lambda, x)$ with accuracy better than about 15% for all $x \geqslant 1.5$. Of course it is only for $x \approx 1.5$ and $\lambda \approx 1$ that our approximation is in error by 15%; normally, it is much better.

For small x, we use the same techniques as in P_1. This means that we will need an approximation to $P_2(\lambda, 0)$ which, unlike $P_1(\lambda, 0)$, is not known analytically. A simple approximation for $P_2(\lambda, 0)$ is

$$P_2(\lambda, 0) = \frac{2\pi\sqrt{2}}{1 + 4(2\pi)^{1/2}\lambda^{3/2} + 2(2\lambda)^{1/2}\lambda^{0.45}} \tag{C17}$$

with a maximum error of 6–7%.

In addition, unlike the $x \geqslant 1.5$ case, where we used the asymptotic expansion (C16) to improve the accuracy, now for large λ there is severe cancellation between $P_2(\lambda, 0)$ and $\int_0^x e^{-\lambda y} \ln(1+y^2) y^{-3/2} dy$, so that it is essential to use Eq. (C16) for $\lambda \geqslant Q_2(x)$, where $Q_2(x)$ specifies beyond what x one should use Eq. (C16). This has been determined as the intersection of the relative error curves for the asymptotic expansion Eq. (C16), which decreases with λ and the logarithm expansion to be discussed below, which increases with λ. A simple expression is

$$Q_2(x) = (0.002157409 + 0.77225089x - 0.245941868x^2)^{-1}, \quad x \geqslant 0.3. \tag{C18}$$

Smaller λ are handled by expanding the logarithm, as for P_1. The error at this intersection is roughly 10%.

For small λ, such that $\lambda x \leqslant 1$, we expand the exponential and obtain, keeping only the first four terms

$$P_2(\lambda, x) = P_2(\lambda, 0) + \lambda x^{1/2}\left[-8 + \frac{4\lambda x}{9} + \frac{4\lambda^2}{15}\left(1 - \frac{x^2}{5}\right)\right] + \frac{\ln(1+x^2)}{x^{1/2}}\left(2 + 2\lambda x - \frac{\lambda^2 x^2}{3} + \frac{\lambda^3 x^3}{15}\right) - 2\sqrt{2}\left(1 + \lambda + \frac{\lambda^2}{6} - \frac{\lambda^3}{30}\right)\ln\frac{1 + x - \sqrt{2x}}{(1+x^2)^{1/2}} - 2\sqrt{2}\left(1 - \lambda + \frac{\lambda^2}{6} + \frac{\lambda^3}{30}\right)[\arctan(1+\sqrt{2x}) + \arctan(\sqrt{2x} - 1)]. \tag{C19}$$

Also, by using Eq. (C9) we obtain

$$P_2(\lambda, x) = P_2(\lambda, 0) - \frac{\gamma\left(\frac{1}{2}, \lambda x\right)}{2\lambda^{3/2}}\left[b_1 + \frac{15}{4\lambda^2}\left[b_2 + \frac{63}{4\lambda^2}\left(b_3 + \frac{143 b_4}{4\lambda^2}\right)\right]\right] + \frac{x^{1/2}e^{-\lambda x}}{\lambda}\left\{b_1 + \frac{15}{4\lambda^2}\left[b_2 + \frac{63}{4\lambda^2}\left(b_3 + \frac{143 b_4}{4\lambda^2}\right)\right] + \frac{x}{\lambda}\left[\left(\lambda x + \frac{5}{2}\right)\left(b_2 + \frac{63}{4\lambda^2}\left(b_3 + \frac{143 b_4}{4\lambda^2}\right)\right) + x^2\left(\frac{9}{2} + \lambda x\right)\left(b_3 + \frac{143 b_4}{4\lambda^2}\right) + b_4 x^4\left(\frac{13}{2} + \lambda x\right)\right]\right\} \tag{C20}$$

with

$$\gamma(a, x) = \Gamma(a) - \Gamma(a, x) \tag{C21}$$

Cancellation is again possible with Eq. (C20) either because $\frac{1}{\lambda}$ is smaller than x, or because even for $\lambda = 0$ the integrand has died before x. This later possibility, however, can only arise for $x \geqslant 1.5$ where we use a different technique, therefore we will once again have to consider only the large λ asymptotic expansions. These asymptotic expansions are different for small x, where Eq. (C16) fails. The source of the problem with Eq. (C16) for small x is that the derivative of $\frac{\ln(1+y^2)}{y^{3/2}}$ diverges as $y \to 0$. This problem cannot be eliminated by integrations by parts, since the higher derivatives will still diverge for small x.

However, for small x (say $x \leqslant 0.1$) and large λ ($\lambda \gg 1$),

$$P_2(\lambda, x) \approx \int_x^1 e^{-\lambda y}\frac{\ln(1+y^2)}{y^{3/2}}\,dy \tag{C22}$$

and using Eq. (C9) we obtain

$$P_2(\lambda, x) \approx \frac{\left\{e^{-\lambda x}\sqrt{x} - e^{-\lambda} + \frac{1}{2\lambda^{1/2}}\left[\Gamma\left(\frac{1}{2}, \lambda x\right) - \Gamma\left(\frac{1}{2}, \lambda\right)\right]\right\}}{\lambda}\left\{b_1 + \frac{15}{4\lambda^2}\left[b_2 + \frac{63}{4\lambda^2}\left(b_3 + \frac{143}{4\lambda^2}\right)\right]\right\} + \frac{e^{-\lambda x}}{\lambda}\left\{b_4 x^{11/2}\left(x + \frac{13}{2\lambda}\right) + \left(x + \frac{9}{2\lambda}\right)x^{7/2}\left(b_3 + \frac{143 b_4}{4\lambda^2}\right) + x^{3/2}\left[x + \frac{5}{2\lambda}\left[b_2 + \frac{63}{4\lambda^2}\left(b_3 + \frac{143}{4\lambda^2}\right)\right] - \frac{e^{-\lambda}}{\lambda}\left\{b_4\left(1 + \frac{13}{2\lambda}\right) + \left(1 + \frac{9}{2\lambda}\right)\left(b_3 + \frac{143 b_4}{4\lambda^2}\right) + \left[1 + \frac{5}{2\lambda}\left(b_2 + \frac{63}{4\lambda^2}\left(b_3 + \frac{143}{4\lambda^2}\right)\right)\right]\right\}\right\}. \tag{C23}$$

This approximation gives an error of 0.25% as $\lambda \to \infty$, which is precisely the difference from b_1 of the correct leading term coefficient in the Taylor expansion of the logarithm, i.e., unity.

The recommended analytical approximations to P_2 are therefore as follows:

For $x \geqslant 1.5$, $P_2(\lambda, x)$ is given by Eq. (C15) if $\lambda < 1$ and by Eq. (C16) otherwise.

For $0.3 < x < 1.5$, $P_2(\lambda, x)$ is given by (C19) if $\lambda \leqslant Q_3(x)$, by (C20) for $Q_2(x) > \lambda \geqslant Q_3(x)$ and by (C16) if $\lambda \geqslant Q_2(x)$.

For $x \leqslant 0.3$, $P_2(\lambda, x)$ is given by (C23) for $\lambda \geqslant 3.843751$, by (C20) for $Q_3(x) < \lambda \leqslant 3.843751$ and by (C19) for $\lambda \leqslant Q_3(x)$.

$Q_3(x)$ specifies the "boundary" between the regions where (C19) and (C20) are best and is determined, as in the case of Q_2, by equating them. A simple approximation for this function is

$$\begin{aligned} Q_3(x) &= 0.6, \quad x \leqslant 0.001 \\ &= \frac{1 + 40.204039698503761x - 14.44217102474144x^2}{2.000637203249082 + 122.2282912572746x - 29.58118497124956x^2}, \quad 0.001 < x < 0.6 \\ &= 0.3, \quad x \geqslant 0.6. \end{aligned} \tag{C24}$$

The maximum error with the recommended approximation is 20% and may be improved if one uses a more refined approximation for $P_2(\lambda, 0)$.

One should emphasize that these approximations are by no means optimal. However, in our view they represent a reasonable compromise between simplicity and accuracy, at least for the purposes of Stark-broadening calculations. For a specific application, such as opacity calculations or scaling laws, one may wish to develop simpler or more accurate approximations, although, in view of the discussion in Sec. 5, we do not see the point in improving the accuracy.

Experience thus far with the present formulas[22] has revealed discrepancies of less than 6% with more exact (dipole) calculations, provided that the minimum impact parameter is such that unitarity is not violated.