Collision operator for isolated ion lines in the standard Stark-broadening theory with applications to the Z scaling in the Li isoelectronic series $3P$-$3S$ transition

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In this work we review some aspects of the semiclassical dipole impact approximation for isolated ion lines with a view to the questions on Z scaling raised by two recent experimental studies. Some theoretical and practical aspects of line-shape calculations are discussed. Detailed calculations are performed in the semiclassical (dipole) impact approximation for the Li isoelectronic $3P$–$3S$ line. Particular emphasis is given to inelasticity effects. In contrast to previous calculations, very good agreement is obtained for the lighter elements of the isoelectronic series. Ion dynamical corrections are also considered and are found to be negligible in the dipole approximation.

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I. INTRODUCTION

Recently some experimental studies [1–3] have found significant deviations from the Z scaling predicted by the impact theory [4–8] for isolated ion lines. The present work makes a detailed study of the $3P$-$3S$ line in the Li-isoelectronic series in the semiclassical (dipole) impact approximation. Quadrupole terms are not considered in detail, although they are known [8,9] to often be important for multiply charged ion emitters. As one can see from the theoretical calculations presented in Refs. [1,2], even within the dipole approximation there is significant disagreement between the different theoretical approaches as well as with experiment. Before one examines higher multipoles (whose contribution can change the Z scaling), it is important to have reached a consensus on the dipole terms. This work stresses the importance of inelasticity in these calculations by calculating the relevant broadening operator exactly (within the semiclassical dipole approximation without resonances).

The paper is organized in four sections. The first section introduces some notation and deals with practical details of a line-shape calculation. The point is not to compare line-shape codes, but to point out some physics of the collision operator that should be included in a general line-shape code and also to point out that such a calculation, even without a fully optimized code, is usually fast enough that no "shortcuts" are needed. The second section applies some of the above results to the case of the experimental results of Refs. [1–3] and shows that the predicted Z scaling is a "simplified" impact theory prediction and valid only under some assumptions. The third section examines the effects of ions and obtains an upper bound for their contribution to the width by calculating ion-dynamical corrections rigorously within the impact approximation. The last section discusses the results of a full calculation (with quasistatic or impact ions) and their implications for the Z scaling.

II. THEORY AND PRACTICAL CONSIDERATIONS

"Conventional" [10–12] line-shape calculations use the impact (or unified) approximation for electrons and the quasistatic one for ions. In the impact approximation [4–8] the line shape $L(\omega)$ is given by

$$L(\omega)=-\frac{1}{\pi}\int dE\, W(E)\mathrm{Re}\mathbf{d}_{\alpha'\beta'}\langle\alpha\beta|[\imath(\omega-\omega_{\alpha\beta})I+\Phi]^{-1}|\alpha'\beta'\rangle\mathbf{d}^{*}_{\alpha\beta}\ . \tag{1}$$

α,α' are states of the initial level and β,β' of the final level involved in the transition in question (in principle they are complete sets of states), Re denotes real part, $W(E)$ is the ionic electric microfield distribution, which is calculated, for example, by APEX [13], I is the unit matrix, $\mathbf{d}$ is the dipole operator, and Φ is a collision operator with matrix elements

$$\begin{aligned}\langle\alpha\beta|\Phi|\alpha'\beta'\rangle=-n\hbar^{-2}\int vf(v)d^{3}\mathbf{v}\int d^{3}\boldsymbol{\rho}\,\delta(\mathbf{v}\cdot\boldsymbol{\rho})\rho\Bigg[\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{t_1}dt_2[\langle\alpha|V'(t_1)|\alpha''\rangle\langle\alpha''|V'(t_2)|\alpha'\rangle\delta_{\beta\beta'}\\ +\delta_{\alpha\alpha'}\langle\beta'|V'(t_1)|\beta''\rangle\langle\beta''|V'(t_2)|\beta\rangle]\\ -\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2\langle\alpha|V'(t_1)|\alpha'\rangle\langle\beta'|V'(t_2)|\beta\rangle\Bigg]\ ,\end{aligned} \tag{2}$$

with n the electron density, $f(v)$ the Maxwell-Boltzman distribution, $V'(t)$ the time-dependent (single) plasma-electron–emitter-electron interaction in the interaction picture, and with α'' and β'' eigenstates of the upper and lower

levels, respectively (in principle they are complete sets of states). Repeated indices are summed over, of course. The δ function assures that the velocity $\mathbf{v}$ and impact parameter $\boldsymbol{\rho}$ satisfy $\mathbf{v}\perp\boldsymbol{\rho}$. The limits of ρ integration are $\rho_{\min}\leq\rho\leq\rho_{\max}$.

The standard values for the two parameters are $\rho_{\max}=0.68\lambda_D$, with λ_D the Debye length and (with a_0 the Bohr radius, $Z_{\rm em}$ the emitter charge, and n_a, n_b the principal quantum numbers of the upper and lower levels, respectively)

$$\rho_{\min}=\max\left[(n_a^2-n_b^2)\frac{a_0}{Z_{\rm em}+1},\sqrt{\tfrac{2}{3}}\frac{\hbar(n_a^2-n_b^2)}{m(Z_{\rm em}+1)v}\right] . \tag{3}$$

If $n_a=n_b$, the difference of their squares should be replaced by n_a^2.

We now introduce some new notation. First, we use a dipole interaction with $\mathbf{E}(t)$ the electric field,

$$V(t)=\mathbf{d}\cdot\mathbf{E}(t)=e\mathbf{r}\cdot\mathbf{E}(t) , \tag{4}$$

where $\mathbf{r}$ is the position vector of the atomic electron. Now we want to separate the purely atomic part (which has the predicted Z scaling) and the part that depends on the details of the collision process. This is, practically speaking, always useful, not just because of the Z-scaling questions. We therefore define two quantities:

$$\phi_d(\omega_1,\omega_2)=-\frac{2\pi ne^2}{3\hbar^2}\int_0^\infty vf(v)dv\int_{\rho_{\min}}^{\rho_{\max}}\rho\,d\rho\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{t_1}dt_2 e^{\iota\omega_1 t_1}e^{\iota\omega_2 t_2}\mathbf{E}(t_1)\cdot\mathbf{E}(t_2) \tag{5}$$

and

$$\phi_{\rm int}(\omega_1,\omega_2)=-\frac{2\pi ne^2}{3\hbar^2}\int_0^\infty vf(v)dv\int_{\rho_{\min}}^{\rho_{\max}}\rho\,d\rho\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2 e^{\iota\omega_1 t_1}e^{\iota\omega_2 t_2}\mathbf{E}(t_1)\cdot\mathbf{E}(t_2) \tag{6}$$

in terms of which (after the angular average)

$$\begin{aligned}\langle\alpha\beta|\Phi|\alpha'\beta'\rangle=&\sum_{\alpha''}\mathbf{r}_{\alpha\alpha''}\cdot\mathbf{r}_{\alpha''\alpha'}\phi_d(\omega_{\alpha\alpha''},\omega_{\alpha''\alpha'})\\&+\sum_{\beta''}\mathbf{r}_{\beta''\beta}\cdot\mathbf{r}_{\beta'\beta''}\phi_d(\omega_{\beta\beta''},\omega_{\beta''\beta})\\&-\mathbf{r}_{\alpha\alpha'}\cdot\mathbf{r}_{\beta'\beta}\phi_{\rm int}(\omega_{\alpha\alpha'},\omega_{\beta'\beta}) .\end{aligned} \tag{7}$$

The question now is the evaluation of ϕ_d (for "direct") and $\phi_{\rm int}$ (for "interference"). Before proceeding, we note Voslamber's [14] valid criticism that the impact (in contrast to the unified) theory is not generally applicable for arbitrary ω_1,ω_2 pairs. We do not discuss this point any further here. Of course, for isolated lines (which is our interest here), $\omega_1=-\omega_2$ and the above criticism does not apply. The evaluation of ϕ_d has been done in the case of isolated ion lines, in the nonshielding limit, using hyperbolic paths for the perturbing electrons by Sahal-Brechot [15], extending the results of Alder *et al.* [16] for a repulsive interaction to the attractive case. Feautrier [17] has further reduced these expressions to integrals over velocity. Calculations of some relevant functions have been done by Klarsfeld [18,19] and *excellent* analytic approximations for the a function of Eq. (9), valid for all parameter ranges, have been given by Poquerusse [20]. Recently, Dimitrijevic and Sahal-Brechot [21] have obtained (also given correctly by Poquerusse's empirical fits) some important asymptotics analytically (there is a $\frac{1}{6}$ factor missing in their expressions for K' due to a typo). Since the derivation of these expressions is not widely known, we outline it in Appendix A.

The net result is that, for isolated lines, $\phi_{\rm int}(\omega_1,-\omega_1)=2\,\mathrm{Re}\phi_d(\omega_1,-\omega_1)=\phi_{\rm int}(\omega_1)$. Let us emphasize again that ϕ is an impact and *not* a unified theory operator, and that the ω *dependence* is an inelasticity dependence. Since the word "inelasticity" is also used with different definitions [22], we define it here to mean that the energy difference between the states connected by a collisionally induced transition cannot be taken approximately equal to 0. With the above relation between the direct and interference terms in mind, we write the final result:

$$\begin{aligned}\phi_{\rm int}(\omega_1,-\omega_1)=&\frac{8\pi n}{3}\left[\frac{e^2}{4\pi\epsilon_0\hbar}\right]^2\left[\frac{2}{\pi}\right]^{1/2}\left[\frac{m}{kT}\right]^{3/2}\\&\times\int_0^\infty dv\,ve^{-mv^2/2kT}[a(\xi_1,\epsilon_{\max}(v))\\&\qquad-a(\xi_1,\epsilon_{\min}(v))] ,\end{aligned} \tag{8}$$

where the function a is given by

$$a(\xi,\epsilon)=e^{\pi|\xi|}|\xi|\epsilon K_{\iota\xi}(|\xi|\epsilon)|K'_{i\xi}(|\xi|\epsilon)| , \tag{9}$$

where $K_{\iota\xi}$ is a modified Bessel function of imaginary order, K' is its derivative with respect to the argument, $\epsilon(v)$ is the eccentricity, given by

$$\epsilon(\rho,v)=\sqrt{1+(\rho/s)^2} \tag{10}$$

with

$$s=\frac{Z_{\rm per}Z_{\rm em}e^2}{4\pi\epsilon_0 mv^2}=\frac{Z_{\rm em}e^2}{4\pi\epsilon_0 mv^2}=\frac{(Z-1)e^2}{4\pi\epsilon_0 mv^2} , \tag{11}$$

where $Z=Z_{\rm em}+1$ is the spectroscopic charge number (i.e., $Z=1$ for neutral species, 2 for singly ionized species, etc.) and ρ is the impact parameter. Hence $\epsilon_{\min}$ is the $\epsilon(v)$ corresponding to the minimum impact parameter

and $\epsilon_{\max}(v)$ corresponds to the maximum impact parameter;

$$\xi_i = \omega_i s / v \tag{12}$$

is a measure of inelasticity.

Numerically speaking, the calculation of (1) requires the calculation of the relevant broadening operator in some basis, a matrix inversion, and an integration over electric microfields. As far as the basis is concerned, we can use a field-independent or a field-dependent basis. A field-independent basis is normally used, as it has the advantage that the collision operator will only need to be evaluated once and for all, and the disadvantage that the quasistatic plasma-emitter interaction can be evaluated to—at best—second order in the self-energy (although in practice only the first order is used), i.e., at most the same order as the collision operator. In practice the advantage of the field-independent basis normally outweighs its disadvantage. As far as the integration goes, excellent results are obtained using say 19 Gaussian quadrature points, covering the integration range from 0 to infinity (using a transformation for high fields to map them onto a finite region) rather than 50 or so as reported by Calisti *et al.* [23]. We use just 15 Gaussian quadrature points for the region from 0 to 9 Holtzmark fields, and 4 fields for the remaining region (with the transformation $E \rightarrow 1/E$). This is hardly surprising: Writing $L(\omega) = \int dE\, W(E) J(\omega, E)$, although, $J(\omega, E)$ as a function of ω, for a particular E field may be sharp, as a function of E, it is quite smooth. We could probably have used even fewer fields. We want to emphasize that (apart from using selection rules [12]) the code is not at all slow for the purposes of calculating a single line. Typical run times for 45–50 frequency points range from at most (including validity checks) a second for a $3P$-$3S$ isolated ion line (such as the transition to be discussed later) to a few minutes for high principal quantum number overlapping neutral lines on a Convex computer. The most time consuming part for the partially overlapping case, i.e., when ω_1, ω_2 are neither opposites nor equal to 0 (this time Voslamber's objections are valid, but we nevertheless want to give an idea of the difficulty in terms of CPU time), is typically the inelastic collision integral calculation, which for a 21×21 (ω_1, ω_2) grid takes about 35 seconds for the partially overlapping neutral line case (and this will be only done once). Further optimization [such as the diagonalization approach of Calisti *et al.* [23,24], which eliminates $N_E \times N_\omega$ inversions (N_E is the number of microfields for the integration and N_ω is the number of frequency points where the line shape is desired) in favor of N_E diagonalizations, plus, if no approximations are made, N_E inversions of the transformation matrix] can drastically reduce execution time. However, some care must be taken in such an approach, as errors in the eigenvectors can sometimes amplify in the calculation of the autocorrelation function.

The main point of the above discussion is that, at least for lines such as the ones considered in Refs. [1–3] [for which (dipole) quasistatic broadening is not important anyway] and for simple applications (excluding opacity calculations, for example), a fully consistent (dipole) impact-theory calculation is not much slower than approaches based on Gaunt factor estimates (as, for example, in Refs. [25–27]). Another popular simplified calculation (for example, Ref. [23]) is along the lines of Ref. [28]: This introduces a collision operator that incorporates some of the inelasticity and is also a unified theory operator, via "Lewis-type" [29] cutoffs.

An important thing to keep in mind in the case of isolated ion lines where the inelasticity must be taken into account is that, as $|\omega_1| \rightarrow \infty$, $\phi(\omega_1)$ (from now on we denote by ϕ the real part of ϕ_d) does not, as one might expect, decay to 0 (or to the strong collision estimate), but tends toward a constant value (plus the strong collision term) if the minimum impact parameter is allowed to go to 0. This is illustrated in Fig. 1. This constant value comes from the small-ϵ region, where the $a(\xi, \epsilon)$ function approaches the constant value $\pi/\sqrt{3} \approx 1.81$ as $\xi \rightarrow \infty$ and $\epsilon \rightarrow 1$. Note that this constant value is by no means negligible. This can be important as far as Z scaling is concerned and is discussed in the next section. In contrast to this behavior, Griem, Blaha, and Kepple's (GBK) [28] method of accounting for inelastic collisions leads to a ϕ operator that decays to 0 for large energy separations. (Let us again emphasize that the energy separations refer to the energy difference of the upper and lower levels from the levels that broaden them, *not* the separation from the line center.) Another point that is relevant here is the "spike" for small ω. That this feature must be there is very easy to see from the A-function expression (Appendix A). It must be mentioned that this "spike" occurs in a (small-ξ) region where the semiclassical Coulomb excitation theory is most valid (large velocities, small energy spacings). Collision operators that are monotonically decreasing with increasing energy spacing are likely to underestimate the width, although how serious this is depends on a number of factors, including the energy spacing and the "width" and height of the "spike."

For neutral and isolated ion lines, it is easy to generate a table of collision operators vs frequency separations and to subsequently interpolate to obtain the actual collision operator. For energy separations that are large enough (outside the range of our tabulated values) we can use the asymptotic collision operator ϕ_{as}, should such a need

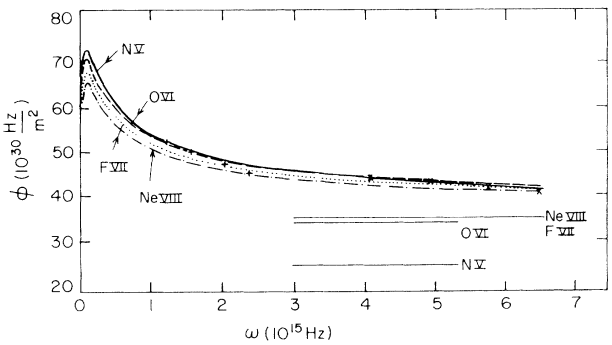

FIG. 1. $\phi(\omega)$ vs energy separation ω, at $n = 1.8 \times 10^{18}$ e/cm^3, $T = 12.5$ eV (as in [1]). Also shown (straight lines) are the asymptotes. + denotes the $3D$-$3P$ and $\times$ the $3P$-$3S$ energy separation.

arise [it need not arise in an actual calculation, but ϕ_{as} may be useful for approximate analytical expressions for $\phi(\omega)$]. The asymptotic limit of ϕ is

$$\phi_{as}=-\frac{4\pi n}{3}\left[\frac{e^2}{4\pi\epsilon_0\hbar}\right]^2\left[\frac{2m\pi}{3kT}\right]^{1/2}(1-e^{-mv_c^2/2kT})+\phi_s\ , \tag{13}$$

where ϕ_s is the strong-collision term (Appendix B) and v_c is defined as, for example, in Kepple [22]:

$$v_c=\left[\frac{3}{2}\right]^{1/2}\frac{\hbar Z(Z-1)}{n_a^2 a_0 m}\ . \tag{14}$$

One must keep in mind that this is a hydrogenic estimate. It is, for example, too pessimistic for ions, and neither is the hydrogenic ρ_{min} unitarity cutoff especially good in the nonhydrogenic case (where it can underestimate the real minimum impact parameter by a factor of 5). Figure 2 illustrates this point.

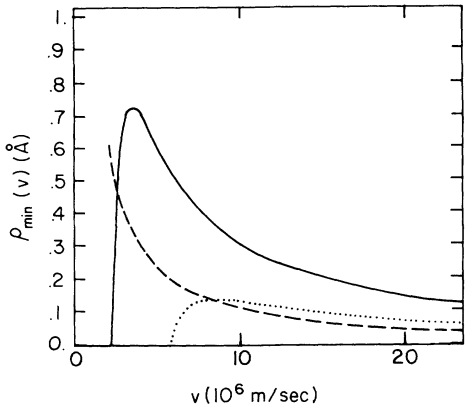

FIG. 2. $\rho_{min}(v)$ vs v for N V; $n=1.8\times10^{18}$ e/cm^3, $T=12.5$ eV. The solid line is unitarity cutoff, the dashed line is "de Broglie" ρ_{min}, and the dotted line is hydrogenic unitarity cutoff. The "wave-function extent" cutoff is 0.95 Å.

In other words, using this cutoff and estimating the minimum impact parameter as

$$\rho_{min}(v)=\frac{[1-(v_c/v)^2]^{1/2}e^2Z_{em}Z_{per}}{4\pi\epsilon_0 mvv_c} \tag{15}$$

violates unitarity (and this happens for a v region that is around the peak of the Maxwell-Boltzmann distribution) and thus overestimates the electron width for C IV at all plasma parameters considered. This is the reason for not including C IV in Fig. 1. For the other species, although the hydrogenic minimum impact parameter is too small, our semiclassical minimum impact parameters used in the error analysis are always larger than the above unitarity-based minimum impact parameter, and thus unitarity violation is covered by our error bounds. This is not true for ion perturbers where unitarity considerations determine the minimum impact parameter over a large velocity range.

For all calculations we have used a self-consistent velocity-dependent minimum impact parameter determined by solving the equation

$$\frac{2}{3}\left[\frac{mv}{\hbar Z_{em}\epsilon}\right]^2\left[\sum_k\frac{\langle 3P^{3/2}\|r\|k\rangle^2}{4}A(\xi(\Delta\omega_k,v),\epsilon)+\sum_j\frac{\langle 3S\|r\|j\rangle^2}{2}A(\xi(\Delta\omega_j,v),\epsilon)\right]-1=0 \tag{16}$$

with $\Delta\omega_k$ and $\Delta\omega_j$ the absolute energy differences of the kth upper-level perturbing state from $3P^{3/2}$ and the jth lower-level perturbing state from the $3S$ state and the A function is defined in Eq. (A33). We also use the correct v_c (i.e., the maximum velocity below which no unitarity violation occurs even for $\rho_{min}=0$) rather than the hydrogenic of Eq. (14); this is to be understood from now on whenever we use v_c.

The asymptotic limit (13) is "reached" when

$$\omega_{as}=\frac{\pi\epsilon_0 m}{e^2Z_{em}}\max\left[32v_l^3,\frac{2v_l^3}{(\eta_1-\arctan\eta_1)},\frac{0.6(3\langle v\rangle)^3\delta(v_c-v_l)}{(\eta_2-\arctan\eta_2)}\right] \tag{17}$$

with

$$\eta_1=[\epsilon^2(\rho_{max},10^{-5}v_l)-1]^{1/2}\ ,$$
$$\eta_2=\sqrt{\epsilon^2\{\rho_{min}[v_l(1+10^{-5})],v_l\}-1}\ , \tag{18}$$

and

$$v_l=\min(v_c,3\langle v\rangle)\ . \tag{19}$$

Appendix B has some details. In practice ω_{as} is very large, reflecting the slow convergence to the asymptotic limit. Numerically, however, this introduces few problems.

This asymptotic behavior, although correct within the semiclassical impact approximation, may be questioned on the grounds that for small impact parameters the semiclassical approximation is questionable. If one then cuts off the impact-parameter integration at some minimum impact parameter, one gets instead a $\phi(\omega)$ that does decay to 0 as $\omega\to\infty$ (but one also gets a strong-collision term, which may be thought of as an uncertainty originating from the unknown strong collision contribution). Within a semiclassical theory, only error bounds

may be obtained for this strong-collision term. Since the energy separation between levels increases with increasing charge, questions on the asymptotic behavior of $\phi(\omega)$ which is determined by the small-ϵ region of $a(\xi,\epsilon)$ are very important for multiply charged ions and these questions cannot be answered conclusively within a semiclassical formalism. For the calculations that follow (as is clear from Appendix B) we have used no minimum impact-parameter cutoff for $v < v_c$, but we have also done calculations with cutoffs, in order to obtain error bounds. We want to emphasize that our operator is a reasonable one in that it does not violate unitarity of the relevant S matrices and is no less justified than any other semiclassical operator. Indeed, to use a semiclassical approach, the errors associated with the cutoffs should be small. We will therefore use this operator for all calculations, supplemented by an error analysis as outlined in Appendix C. In Fig. 3 we compare some collision operators for N V, Ne VIII, and O VI for some plasma conditions of the experiments of Ref. [2]. The hydrogenic limit of GBK is of course higher, since GBK corresponds to a straight-line-path formalism and assumes that the minimum cutoff is due to the finite wave-function extent, both of which are reasonable assumptions for ICF-type plasmas, for which this operator was proposed. For the experiments of Refs. [1–3], however, the conditions are far from ICF-type conditions and the use of the GBK operator may be problematic. The Dimitrijevic-Konjevic (DK) operator is also very different from ours for large energy separations.

Since complete profile calculations for, say, the $3P$-$3S$ lines of Refs. [1–3] are fast for our purposes, we use the exact semiclassical operator instead of semiempirical formulas. Once one has an impact operator, one can use the method of GBK to construct an approximate (unified theory) frequency-dependent collision operator, in the Lewis cutoff spirit, but without the discontinuities involved in the original Lewis cutoff method.

III. Z-SCALING PREDICTIONS OF THE IMPACT THEORY

The impact theory is "supposed to" (that is, if we neglect inelasticity considerations) predict [1,2] a Z^{-2} scaling. This is easy to understand, since the width and shift operator in the impact or unified theories that use a dipole atom-plasma interaction is proportional to $\mathbf{d}\cdot\mathbf{d}$, with $\mathbf{d}$ the atomic dipole operator. Since the Bohr radius goes as $1/Z$, we expect the Z^{-2} scaling. We have checked this assumption by graphing the quantity $\sqrt{f\Delta\lambda}$ for the $3p$-$3s$ and $3p$-$3d$ oscillator strengths f vs Z^{-1} for lithiumlike carbon, nitrogen, oxygen, fluorine, and neon. Data were taken from Lindgard and Nielsen [30] and Wiese, Smith, and Glennon [31] and also from Cowan's code [32]. To expect Z^{-2} scaling, these should be proportional to $1/Z$, as these are proportional to the reduced matrix elements in question. Proportionality to $1/Z$ was very well satisfied (to better than 0.6% in all cases). Quadrupole and higher multipole interactions should be important only for the more highly charged ions, thus increasing their widths from the simple $1/Z^2$ prediction and making the overall scaling more like $1/Z$. As men-

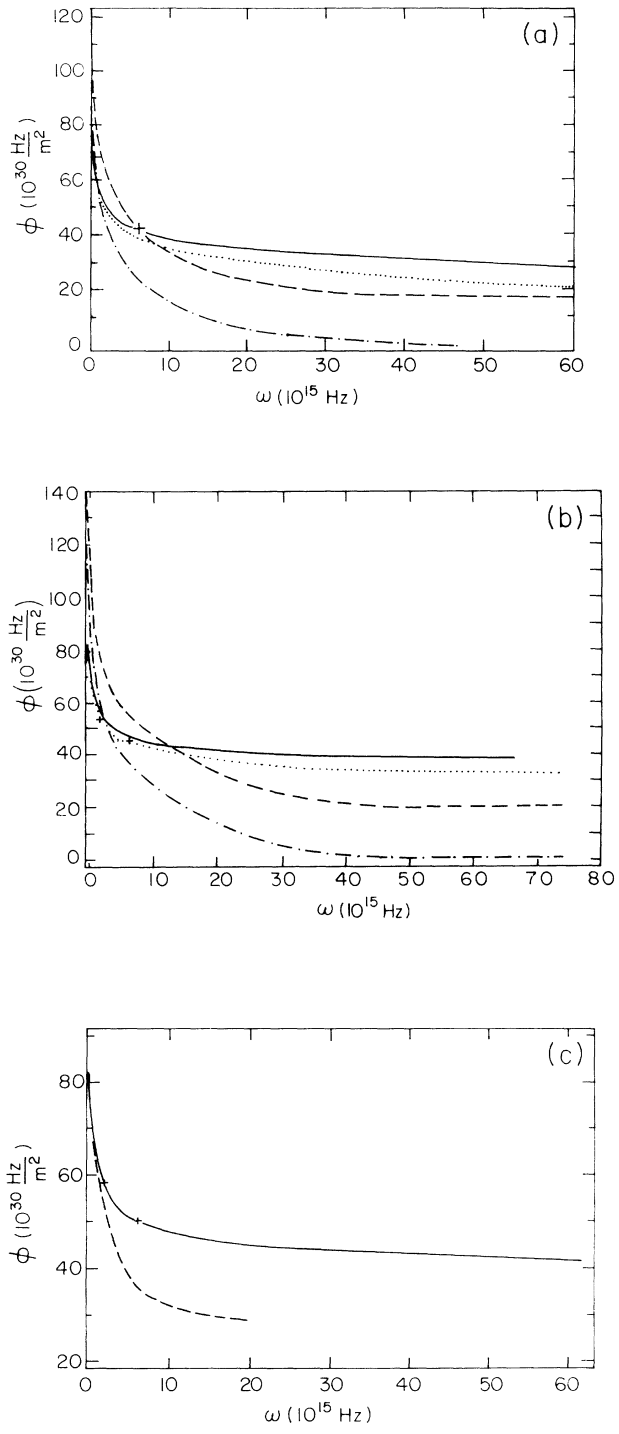

FIG. 3. $\phi(\omega)$ vs energy separation ω. (a) N V: $n = 2.3\times10^{18}$ e/cm^3, $T = 23.9$ eV; (b) Ne VIII: $n = 2.8\times10^{18}$ e/cm^3, $T = 29.7$ eV; (c) O VI; $n = 2.4\times10^{18}$ e/cm^3, $T = 17.5$ eV. For (a) and (b) the solid line is the collision operator without $\rho_{\min}$ cutoff except for $v > v_c$, the dotted line is with cutoff as in Appendix C, the dashed line is GBK with the strong-collision term, and the dash-dotted line is GBK without the strong-collision term. For (c) the solid line is the collision operator with only the unitarity cutoff for $v > v_c$ and the dashed line is the operator of Dimitrijevic and Konjevic. The relevant energy separations are marked by +.

tioned in the Introduction, however, we will not consider quadrupole interactions in detail here.

Within the impact theory there is another factor which can change the simple Z^{-2} prediction, namely, inelasticity of collisions. As Fig. 1 shows, it is very important in which part of the $\phi(\omega)$ vs ω curve the relevant (e.g., $3D$-$3P$ and $3P$-$3S$) energy separations lie. Apart from the fact that even the hydrogenic ($\omega=0$) limit is not exactly the same due to different $Z_{\rm em}$, deviations may be expected since the relevant energy separations are not the same for different species. If they all fall in the "flat" (i.e., large-ω) region, then we might expect only small deviations from the Z^{-2} scaling. If, however, for at least one species these energies fall in the steep part of the curve, we may expect significant deviations. Referring to the graphs of Fig. 1, we see that N V gains approximately 5%, 10%, and 14% relative to O VI, F VII, and Ne VIII, respectively, as far as the $3D$-$3P$ channel is concerned. For the $3P$-$3S$ channel these numbers are approximately 2%, 5%, and 6%, respectively. This, of course, changes the Z scaling in a direction *opposite* to the one needed to explain the observed scaling. So, while the inelasticity contribution to the Z scaling cannot account for the observed discrepancies, it should be kept in mind that the Z^{-2} scaling is a "simplified" and *not* a rigorous impact-theory prediction. This effect may also affect the temperature scaling, as different temperatures lead to different rates of decrease of the $\phi(\omega)$ operator.

IV. ION BROADENING

Here we address the question of whether broadening due to ion perturbers may be important in explaining the results of Refs. [1–3]. The criterion for quasistatic behavior of the ions is that the combined effect of all other broadening mechanisms (e.g., electron collisions, Doppler, quasistatic ions) is large enough as to have caused appreciable "memory loss" (i.e., the autocorrelation function has decayed appreciably, for example, well below the $1/e$ level) in a time short enough that the ions have not moved appreciably. In other words (and neglecting Doppler and quasistatic broadening which are unimportant in our case), for the ions to be quasistatic, the density must be high enough or the temperature low enough that electron collisions are strong enough that their cumulative effect can cause memory loss in a time short enough that the ions have not moved appreciably. Forgetting for the moment any other considerations, there is therefore reason to expect an increase in the importance of ion-dynamical effects for the more highly ionized ions of the isoelectronic series because they are more compact (hence less polarizable) due to the extra attraction on the wave functions, and therefore interact more weakly with the plasma and lose memory more slowly (thus giving ions time to move).

First, it is easy to see that the ions are *not* quasistatic, since even the necessary *although generally insufficient* criterion [33]

$$w^{1/2} > (2kT/\mu)^{1/2}/\rho_0 \tag{20}$$

with $w^{1/2}$ the half width at half maximum (HWHM), μ the reduced ion-radiator mass, and ρ_0 the average interionic spacing is not even close to being fulfilled. This rules out any thoughts of attributing the observed discrepancies to quasistatic ion quadrupole broadening [2]. Second, it is possible to see that ion dynamics will not be important here. For this reason we have done an impact calculation with "reduced" protons. In fact Griem [34] has argued (neglecting the dipole contribution in the minimum impact parameter) that ions are "impact" for the plasma conditions of interest in Refs. [1–3]. Whether or not the impact approximation is valid for these protons is irrelevant if it turns out that the proton-impact width is much smaller than the electron impact width, since (by virtue of being linear in the density) the impact width is the largest attainable width at a given density and temperature (in the impact approximation each collision contributes to an additive manner to "memory loss"). The reason for the fact that the ion broadening is small is a combination of the hyperbolic path and the inelasticity. Mathematically speaking, the repulsive (dipole interaction) $a(\xi,\epsilon)$ function is obtained by multiplying the attractive one by $e^{-2\pi|\xi|}$. When $\omega\rightarrow 0$ (hydrogenic or "collisionally degenerate" [14(b)] case) there is no difference and consequently the velocity integration gives a much larger ϕ than for electrons. However, unlike the electron case, the a function decays to 0 rapidly for large ω and so does $\phi(\omega)$. (This decay depends in a very sensitive manner on the temperature.) It turns out that the ionic ϕ at the frequencies of interest, i.e., the $3D$-$3P$ and $3P$-$3S$ energy separations, are smaller than the electronic ones. In the cases examined here, the ionic ϕ for the $3P$-$3S$ energy separation which gives the main contribution is always completely negligible compared to the electronic one. The reason for this was explained above and should be kept in mind: The fact that ions may not be efficient for broadening ion lines compared to electrons is (as we saw by considering the $\omega=\xi=0$ result) mainly an inelasticity (i.e., $\xi\neq 0$) effect; it may be misleading to attribute it to the Coulomb repulsion weakening the effective interaction [9], since the Coulomb repulsion is not strong enough to prevent the ions from entering the Debye sphere. It is true that the Coulomb field deflects the incoming ions, but it also slows them down (thus making the collision stronger) and these effects tend to cancel. It is quite possible that for higher temperatures (since the Maxwell-Boltzmann distribution is shifted to the right and higher v's are more probable, resulting in smaller ξ's) or lighter elements (which have smaller energy spacings), the ionic ϕ will decrease at a slower rate and thus compete or even dominate the broadening, as the rate of decrease of the ionic $\phi(\omega)$ is critical. Figure 4 and Tables I and II illustrate this point.

One may see that in all cases the ionic ϕ is much less than the electronic one. Also, the strong-collision contribution from ions is negligible.

Summing up, there are two factors which could make the results deviate from the $1/Z^2$ scaling in the direction of increasing the relative widths of the higher members: These factors are higher multipole corrections and ion dynamics. The present calculations show that while the

TABLE I. Electron vs proton impact $\phi(\omega)$ [1].

Species	Transition	ϕ_{el} (10^{30} Hz/m^2)	ϕ_{ion} (10^{30} Hz/m^2)
C IV	3*D*-3*P*	51	0.28
C IV	3*P*-3*S*	37	1.1×10^{-7}
N V	3*D*-3*P*	53	0.13
N V	3*P*-3*S*	44	1.9×10^{-7}
O VI	3*D*-3*P*	50	0.05
O VI	3*P*-3*S*	43	2×10^{-7}

ionic contribution should in general be investigated, the more so as it is sensitive to temperature (higher temperature means smaller ξ), it is not important for the experiments of Refs. [1–3], in agreement with Blaha's results [9]. Ionic collisions can only be important at higher temperatures and smaller energy spacings. We emphasize that we have only shown that the *dipole* contribution of ion dynamics is not important; for the quadrupole contribution, the $\xi=0$ channel is always available. Since in that case there is no exponential damping (e.g., exponents with arguments proportional to $-\xi$) in the relevant functions, the ionic quadrupole contribution could in principle be larger than the electronic one (see Ref. [18] for the relation between the attractive and repulsive quadrupole functions).

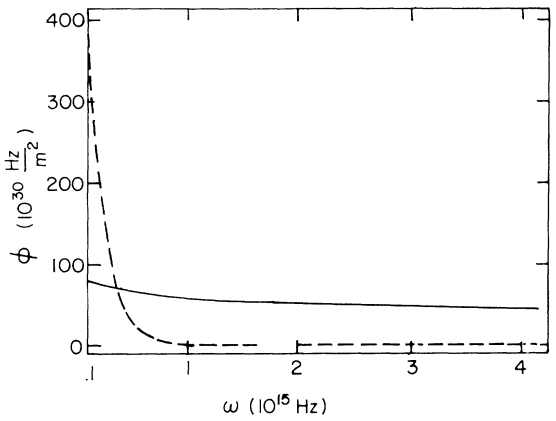

FIG. 4. Electronic vs ionic $\phi(\omega)$. N V: $n=2.3\times10^{18}$ e/cm^3, $T=23.9$ eV. Electronic is shown by the solid line and ionic is shown by the dashed line.

V. RESULTS AND DISCUSSION

We have performed calculations using the full inelastic calculation for the width functions only. We have not modeled the shift, partly because it is believed to be small and partly because it was not considered in Refs. [1–3]. It may be of some importance for the C IV lines. The fol-

TABLE II. Electron vs proton impact $\phi(\omega)$ [2,3].

Species	kT (eV)	n_e(10^{18} e/cm^3)	Transition	ϕ_{el} (10^{30} Hz/m^2)	ϕ_{ion} (10^{30} Hz/m^2)
C IV	7.0	1.5	3*D*-3*P*	50.4	0.05
C IV	7.0	1.5	3*P*-3*S*	37.7	2.4×10^{-9}
C IV	8.6	2.4	3*D*-3*P*	75.8	0.15
C IV	8.6	2.4	3*P*-3*S*	56.1	1.5×10^{-8}
N V	14.9	1.2	3*D*-3*P*	33.3	0.145
N V	14.9	1.2	3*P*-3*S*	27.6	3.5×10^{-7}
N V	18.7	1.6	3*D*-3*P*	41.5	0.33
N V	18.7	1.6	3*P*-3*S*	33.9	1.6×10^{-6}
N V	21.8	2.0	3*D*-3*P*	49.6	0.57
N V	21.8	2.0	3*P*-3*S*	40.2	4.8×10^{-6}
N V	23.9	2.3	3*D*-3*P*	55.6	0.79
N V	23.9	2.3	3*P*-3*S*	44.6	9×10^{-6}
O VI	8.3	1	3*D*-3*P*	31.4	0.004
O VI	8.3	1	3*P*-3*S*	27.9	7.0×10^{-9}
O VI	11.5	1.3	3*D*-3*P*	37	0.028
O VI	11.5	1.3	3*P*-3*S*	32.23	0.9×10^{-7}
O VI	15.6	2.1	3*D*-3*P*	54.8	0.14
O VI	15.6	2.1	3*P*-3*S*	47	9.6×10^{-7}
O VI	18.5	2.4	3*D*-3*P*	60.69	0.23
O VI	18.5	2.4	3*P*-3*S*	51.58	2.1×10^{-6}
F VII	14.4	1.57	3*D*-3*P*	40	0.035
F VII	14.4	1.57	3*P*-3*P*	34.8	4.9×10^{-7}
F VII	16.6	2.1	3*D*-3*P*	51	0.085
F VII	16.6	2.1	3*P*-3*S*	44.3	1.6×10^{-6}
F VII	18.5	2.92	3*D*-3*P*	68.8	0.18
F VII	18.5	2.92	3*P*-3*S*	59.5	4.21×10^{-6}
Ne VIII	29.7	2.8	3*D*-3*P*	55.86	0.519
Ne VIII	29.7	2.8	3*P*-3*S*	47.4	3.27×10^{-5}
Ne VIII	42.5	3.2	3*D*-3*P*	58.36	1.45
Ne VIII	42.5	3.2	3*P*-3*S*	49	2.26×10^{-4}

lowing levels have been included: $3S$, $3P^{1/2}$, $3P^{3/2}$, $3D^{5/2}$, $3D^{3/2}$, $4D^{3/2}$, and $4D^{5/2}$. All of them are allowed to participate in upper-level broadening, while only the first three were allowed to participate in lower-level broadening.

If the collision operator does not vanish in the limit of large energy separations, these are questions on the applicability of the "no quenching" assumption normally employed. This is why we have dropped this assumption and included the $4D$-$3P$ channel. For example, the relative contribution of the $4D$-$3P$ transition compared to the combined contribution of the $3P$-$3D$ and $3S$-$3P$ transitions is estimated from the ratio of the squares of the reduced matrix elements times the ratio of the $\phi(\omega)$ values from Fig. 1. For all species considered, this ratio is less than 10%. It must be mentioned, however, that this contribution is uncertain because the energy transfer involved is of the order of the electron's kinetic energy for the $4D$-$3P$ energy separation, so a classical path assumption is questionable. The reduced matrix elements for other channels are too small to be considered.

As for the strong-collision contribution, although much effort has been put into obtaining better estimates for it, we still take Baranger's point of view that if the strong-collision term is important, the calculation is not reliable. Consequently we still use the Lorentz-Weisskopf estimate, divided by 2 in order to bring it closer to Griem's estimate. In fact, in the framework of this calculation which uses no minimum impact-parameter cutoff other than what is needed (for $v > v_c$) to preserve unitarity, the strong-collision term for the dipole interaction alone is of the order of 1%. A better treatment of the strong-collision contribution was done as outlined in Appendix C and this results in the error bars of Table III.

Oscillator strengths taken from Wiese, Smith, and Glennon [31] have been used to calculate the relevant N V and O VI reduced matrix elements, i.e., the program accepts oscillator strengths (it also accepts radial matrix elements, if they are available) and calculates the reduced matrix elements. For F VII and Ne VIII energies and oscillator strengths have been taken from Cowan's [32] code. Generally speaking, calculating reduced matrix elements from oscillator strengths is incorrect, since the sign of the reduced matrix elements need not be positive. In the case of isolated lines, however, this makes no difference. The results are tabulated below for comparison with experiment. We only compare with Refs. [2] and [3], as these are the most accurate results, as a result of a number of improvements [2] over Ref. [1]. The Doppler effect has been accounted for in the calculations via the usual convolution procedure (done analytically after a spline interpolation of the pure Stark spectra), although it makes very little difference. In the rightmost column we list widths after the convolution and then (in parentheses) the pure Stark widths with error bars. As far as these error bars are concerned, they are calculated with a (velocity-dependent) cutoff at

$$\rho_{\min}=\max\left[\frac{b\hbar}{mv},\frac{n_a^2 a_0}{Z},\rho_u(v)\right] \tag{21}$$

as in Appendix C, with $b=1$ (significantly higher values for b starting raising doubts about the validity of the semiclassical approach) and $\rho_u(v)$ is obtained by solving (16). The lowest bound corresponds to a strong-collision contribution of 0 and the highest to the replacement of $\{S_a S_b - 1\}$ by -1 (-2 would be the absolute maximum). We must also point out that the error bounds given take the density and temperature values as certain and do not incorporate errors from the experimental density-temperature determination.

For F VII and Ne VIII the calculated widths are smaller and the discrepancies are particularly serious for Ne VIII. One might observe that some calculated widths are very close to the lower bounds. This is not an accident and it is related to the fact that $\phi(\omega)$ at the relevant frequencies with cutoff is not too different from the one with no cutoff (see also Fig. 3): It is easy to see that for large energy separations the contribution to $\phi(\omega)$ comes from the region

TABLE III. Theory vs experiment [2,3].

Species	kT_e (eV)	n_e (10^{18} e/cm^3)	FWHM (Å) Expt.	FWHM (Å) Theor.
C IV	7.0	1.5	6.7 ±0.4	7.17(7.17+1.6 or −0.25)
C IV	8.6	2.4	9.7 ±0.5	10.6(10.6+2.4 or −0.31)
N V	14.9	1.2	2.2 ±0.1	2.3(2.13±0.1)
N V	18.7	1.6	2.7 ±0.1	2.7(2.62±0.15)
N V	21.8	2.0	3.4 ±0.2	3.2(3.12±0.2)
N V	23.9	2.3	3.8 ±0.2	3.5(3.47+0.27 or −0.22)
O VI	8.3	1.0	1.0 ±0.1	1.03(1.03±0.035)
O VI	11.5	1.3	1.4 ±0.1	1.25(1.2±0.05)
O VI	15.6	2.1	1.8 ±0.3	1.8(1.74+0.08 or −0.1)
O VI	17.5	2.4	2.1 ±0.2	1.98(1.91+0.09 or −0.12)
F VII	14.4	1.57	0.87±0.1	0.76(0.686+0.05 or −0.026)
F VII	16.6	2.1	1.11±0.13	0.94(0.87+0.07 or −0.04)
F VII	18.5	2.92	1.49±0.18	1.23(1.17+0.12 or −0.03)
Ne VIII	29.7	2.8	1.2 ±0.1	0.66(0.55+0.07 or −0.03)
Ne VIII	42.5	3.2	1.2 ±0.1	0.70(0.56+0.09 or −0.04)

$$\left[v \leq \frac{5\omega(Z-1)e^2}{4\pi\epsilon_0 m} \right]^{1/3} \tag{22}$$

as is clear from Appendix B ($\xi \geq 0.2$). The differences between the calculation with and without cutoff are more serious for a fixed energy separation the smaller the Z (since then $\rho_{\min}$ is largest). Also the smaller the energy separation, the less the relative contribution of the small-ϵ, large-ξ region.

For C IV we have two overlapping Lorentzians and the central portion of the profile is raised more than the wings of the entire profile (i.e., the wings away from the overlapping region) and this results in a decrease of the width. Thus, because of both the overlapping effect and the fact that strong collisions are more important (which leads to a reduction of the weak-collision phase space and therefore ϕ), the effect described in Sec. III is "masked." The profile produced by the program is narrower than a hand calculation based on Eq. (20), which is what would enter into a Z-scaling comparison (and what we give in Table III). Note that a self-consistent minimum impact parameter is particularly important here and its neglect will lead to too large a prediction for the width (which would be hard to explain, as almost any additional mechanism will increase the width).

Summing up, we obtain very good agreement with the experimental data of Ref. [2] for all lines of the lighter species (carbon, nitrogen, and oxygen) and even for F VII the calculated and experimental widths lie within the error bars, although the calculated widths seem to be systematically lower. For the lighter species, our results as well as the experimental results are also in agreement with the recent calculations of Dimitrijevic and Sahal-Brechot, where available [35]. For Ne VIII, agreement is poorer.

As far as scaling is concerned, and leaving Ne VIII aside, the good agreement achieved suggests that our calculation would also match the experiment well at the "comparison" parameters $T=12.5$ eV, $n_e=1.8\times10^{18}$ e/cm^3. We have thus calculated widths at the "comparison" parameters and compared the quantity $\mathcal{W}(Z/\lambda)^2$ for the various species, with $\mathcal{W}$ the FWHM in Å. The largest discrepancy was obtained between N V and Ne VIII with N V about 6% wider. However, $\phi(\omega)$ at the dominant $3P$-$3S$ energy separation was also about 6% larger for N V. For C IV we obtain a $\mathcal{W}(Z/\lambda)^2$ which is about 11% smaller than Ne VIII and 16% smaller than N V. This is due to the unitarity considerations explained in Sec. II, namely, that a large part of the available phase space gives rise to strong collisions that would have violated unitarity. Still, within the error bars, C IV can in fact be even larger than N V.

On an ending note, we want to address the question of approximate quick and easy to use formulas for the collision operator. Consider the $3P^{1/2}\rightarrow 3S$ line with the states $3S$, $3P$, $3D$, and $4D$. In this case we have the following explicit formula for the linewidth (FWHM):

$$\mathcal{W}=\phi(\omega_1)R_1^2+\phi(\omega_2)(2R_2^2+R_3^2)+\phi(\omega_3)R_4^2 , \tag{23}$$

where

$$R_1=\langle 3D^{3/2}\|r\|3P^{1/2}\rangle , \tag{24}$$

$$R_2=\langle 3P^{1/2}\|r\|3S^{1/2}\rangle , \tag{25}$$

$$R_3=\langle 3P^{3/2}\|r\|3S^{1/2}\rangle , \tag{26}$$

$$R_4=\langle 3P^{1/2}\|r\|4D^{3/2}\rangle , \tag{27}$$

and ω_1 is the $3D$-$3P$, ω_2 the $3P$-$3S$, and ω_3 the $4D$-$3P$ energy separations. (The reduced matrix elements R_1-R_4 used may differ by a factor of $4\pi/3$ from the conventional ones and are defined as $[3\hbar f(2J_L+1)/2m\Delta\omega]^{1/2}$ with f the oscillator strength, J_L the lower level J, and $\Delta\omega$ the frequency separation.) Calculations with the above formulas give the same results as Table III. For example, for the highest density O VI results, $R_1=1.028$ Å, $R_2=0.8855$ Å, $R_3=1.25$ Å, $R_4=0.717$ Å, $\phi(\omega_1)\approx 60.7\times10^{30}$ Hz/m^2, $\phi(\omega_2)\approx 51.6\times10^{30}$ Hz/m^2, and $\phi(\omega_3)\approx 42.5\times10^{30}$ Hz/m^2. This gives a (pure Stark) FWHM of 1.9 Å in agreement with the results of Table III, which are also in fair agreement with Ref. [2].

As far as simple formulas are concerned, we believe that the collision operator $\phi(\omega)$ could be better represented. If we know the high-frequency asymptotics and the hydrogenic limit, it is not hard to approximate $\phi(\omega)$ by a function of the form

$$\phi(\omega)=\phi_{\text{as}}+[\phi(\omega=0)-\phi_{\text{as}}]f(\omega) , \tag{28}$$

where f is a function that is unity at $\omega=0$ and vanishes for large ω. The simplest approximation to f, e.g., $f(x)=e^{-Tx}$ with appropriately chosen T, may be a reasonable choice. Of course this is a rough approximation, missing the "spike" at small ω, and better choices of f are possible. Such analytic approximations may be valuable in cases where speed is essential as, for example, in opacity calculations.

Of course one must keep in mind that the operator used here does not account for higher multipoles and resonances, which can be important. Work on the calculation of quadrupole contributions along the lines of Appendix A is in progress.

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APPENDIX A: OUTLINE OF THE DERIVATION OF THE INELASTIC COLLISION OPERATOR

Initially we work on the collision plane (x and y axes) and parametrize the trajectory:

$$x = s(\epsilon - \cosh u) , \tag{A1}$$

$$y = s\sqrt{\epsilon^2 - 1}\sinh u , \tag{A2}$$

$$R = s(\epsilon\cosh u - 1) , \tag{A3}$$

$$t = \frac{s}{v}(\epsilon\sinh u - u) , \tag{A4}$$

with s defined in (11). It may be easily verified that this parametrization correctly describes the trajectory.

The coordinates in the collision frame (primed) are related to the coordinates in this reference frame (unprimed) by the Euler angles; i.e., by the transformation

$$R'(t) = AR(t) = A\begin{bmatrix} x(t) \\ y(t) \\ 0 \end{bmatrix} , \tag{A5}$$

where A is the rotation matrix

$$A = \begin{bmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{bmatrix} \tag{A6}$$

with ϕ in $(0,2\pi)$, θ in $(0,\pi)$, and ψ in $(0,2\pi)$.

We thus have

$$R'(t) = \begin{bmatrix} (\cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi)x(t) + (\cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi)y(t) \\ -(\sin\psi\cos\phi + \cos\theta\sin\phi\cos\psi)x(t) + (-\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi)y(t) \\ \sin\theta\sin\phi x(t) - \sin\theta\cos\phi y(t) \end{bmatrix} . \tag{A7}$$

Thus when we evaluate Φ with $\{\ \}$ denoting plasma average, we get a Φ of the form

$$\Phi = -\left[\frac{e}{4\pi\epsilon_0\hbar}\right]^2 \int dt_1 \int dt_2 e^{\iota\omega_1 t_1} e^{\iota\omega_2 t_2} n \int v f(v) dv \int \rho\, d\rho \sum_{\mu,\nu} d_\mu d_\nu \left\{ \frac{R_\mu(t_1)}{|R(t_1)|^3} \frac{R_\nu(t_2)}{|R(t_2)|^3} \right\}_{\text{an}} . \tag{A8}$$

When we do the angular average $\{\ \}_{\text{an}}$ we get a factor of 2π from the fact that if we take a trajectory in the collision frame and rotate it by any angle, we should get the same contribution and another factor of

$$[x(t_1)x(t_2) + y(t_1)y(t_2)]\frac{\delta_{\mu\nu}}{3} , \tag{A9}$$

where x and y are the axes in the collision plane; hence

$$\{R_\mu(t_1)R_\nu(t_2)\} = \frac{2\pi\delta_{\mu\nu}}{3}[x(t_1)x(t_2) + y(t_1)y(t_2)] . \tag{A10}$$

Thus we get a Φ of the form

$$\Phi = -\frac{2\pi n}{3}\left[\frac{e}{4\pi\epsilon_0\hbar}\right]^2 \mathbf{d}\cdot\mathbf{d} \int v f(v) dv \int \rho\, d\rho \int dt_1 \int dt_2 e^{\iota\omega_1 t_1} e^{\iota\omega_2 t_2} \frac{x(t_1)x(t_2) + y(t_1)y(t_2)}{R^3(t_1)R^3(t_2)} . \tag{A11}$$

From now on we replace x, y, t, and R by their parametrizations in terms of u and obtain (note that $dt = R\,du/v$)

$$\Phi = -\frac{2\pi n}{3}\left[\frac{m}{e\hbar Z_{\text{ion}}}\right]^2 \mathbf{d}\cdot\mathbf{d} \int_0^\infty v^3 f(v) dv \int_{\rho_{\min}}^{\rho_{\max}} \rho\, d\rho \int du_1 \int du_2 e^{\iota\omega_1 s(\epsilon\sinh u_1 - u_1)/v} e^{\iota\omega_2 s(\epsilon\sinh u_2 - u_2)/v}$$

$$\times \frac{(\epsilon - \cosh u_1)(\epsilon - \cosh u_2) + (\epsilon^2 - 1)\sinh u_1 \sinh u_2}{(\epsilon\cosh u_1 - 1)^2(\epsilon\cosh u_2 - 1)^2} . \tag{A12}$$

The quantities we want to evaluate are thus of the form

$$\phi(\omega_1,\omega_2) = \frac{-2\pi n}{3}\left[\frac{e^2}{4\pi\epsilon_0\hbar}\right]^2 \left[\frac{2}{\pi}\right]^{1/2} \left[\frac{m}{kT}\right]^{3/2} \int_0^\infty dv\, v e^{-mv^2/2kT} \int_{\epsilon_{\min}(v)}^{\epsilon_{\max}(v)} d\epsilon\, \epsilon G(\xi_1,\xi_2,\epsilon) , \tag{A13}$$

where for the direct terms we have

$$G(\xi_1,\xi_2,\epsilon) = \int_{-\infty}^{\infty} du_1 \int_{-\infty}^{u_1} du_2 e^{\iota\xi_1(\epsilon\sinh u_1 - u_1)} e^{\iota\xi_2(\epsilon\sinh u_2 - u_2)} \frac{(\epsilon - \cosh u_1)(\epsilon - \cosh u_2) + (\epsilon^2 - 1)\sinh u_1 \sinh u_2}{(\epsilon\cosh u_1 - 1)^2(\epsilon\cosh u_2 - 1)^2} \tag{A14}$$

and for the interference terms we have

$$G(\xi_1,\xi_2,\epsilon)=\int_{-\infty}^{\infty}du_1\int_{-\infty}^{\infty}du_2 e^{\iota\xi_1(\epsilon\sinh u_1-u_1)}e^{\iota\xi_2(\epsilon\sinh u_2-u_2)}\frac{(\epsilon-\cosh u_1)(\epsilon-\cosh u_2)+(\epsilon^2-1)\sinh u_1\sinh u_2}{(\epsilon\cosh u_1-1)^2(\epsilon\cosh u_2-1)^2}\ . \tag{A15}$$

Numerically it is hard to obtain G from its definition because there is a singularity at $\epsilon=1$.

1. Interference terms

For the interference terms, G is purely real and may be written as

$$G(\xi_1,\xi_2,\epsilon)=\frac{1}{\epsilon^2}\left[G_1(\xi_1,\epsilon)G_1(\xi_2,\epsilon)+\frac{\epsilon^2-1}{\epsilon^2}G_2(\xi_1,\epsilon)G_2(\xi_2,\epsilon)\right] \tag{A16}$$

with

$$G_1(\xi,\epsilon)=\int_{-\infty}^{\infty}du\frac{e^{\iota\xi(\epsilon\sinh u-u)}\left[1-\frac{\cosh u}{\epsilon}\right]}{(\cosh u-1/\epsilon)^2} \tag{A17}$$

and

$$G_2(\xi,\epsilon)=\int_{-\infty}^{\infty}du\,\sinh u\frac{e^{i\xi(\epsilon\sinh u-u)}}{(\cosh u-1/\epsilon)^2}\ . \tag{A18}$$

We now evaluate these two functions. Two tricks are involved (as in Alder *et al.* [16]): (a) to avoid violent oscillations in the exponential, we deform the contour so that we have a decaying exponential; and (b) we do a partial integration to make the integrand less singular. In fact, when $\epsilon\to1$ we get a singularity from $u_1=0$ and $u_2=0$ if we try to do the integral as it is.

Symmetry properties of G_1 and G_2

For G_1, since everything else is even (only the cosine will contribute),

$$G_1(\xi,\epsilon)=G_1(|\xi|,\epsilon)\ , \tag{A19}$$

and for G_2, since only the sine will contribute,

$$G_2(\xi,\epsilon)=-G_2(-\xi,\epsilon)=\mathrm{sgn}(\xi)G_2(|\xi|,\epsilon)\ . \tag{A20}$$

We thus only need to deal with positive ξ.

Evaluation of G_2

G_2 may be evaluated simply. First note that

$$\frac{d}{du}\left[-\frac{1}{\cosh u-1/\epsilon}\right]=\frac{\sinh u}{(\cosh u-1/\epsilon)^2}\ . \tag{A21}$$

Hence, when we do a partial integration, the surface term vanishes and we get

$$G_2(\xi,\epsilon)=\iota\xi\epsilon\int_{-\infty}^{\infty}du\ e^{\iota\xi(\epsilon\sinh u-u)}\ . \tag{A22}$$

[Observe that (A20) is satisfied.] We now consider only positive ξ and evaluate

$$I=\oint_C dz\ e^{\iota\xi(\epsilon\sinh z-z)}=0 \tag{A23}$$

since there are no singularities inside the contour C, which consists of the rectangular piece (traversed counterclockwise) $-R\le x\le R$, $y=0$, $x=R$, $0\le y\le\pi/2$, $-R\le x\le R$, $y=\pi/2$, and $x=-R$, $0\le y\le\pi/2$, with $z=x+\iota y$. Eventually we take the limit $R\to\infty$. The vertical sides do not contribute and we get

$$\begin{aligned}G_2(\xi,\epsilon)&=2\iota\xi\epsilon e^{|\xi|\pi/2}\int_0^{\infty}du\ e^{-|\xi|\epsilon\cosh u}\cos\xi u\\&=2\iota\xi\epsilon e^{|\xi|\pi/2}K_{\iota|\xi|}(|\xi|\epsilon)\ .\end{aligned} \tag{A24}$$

Equation (A24) may be written as

$$G_2(\xi,\epsilon)=2\iota\xi\epsilon e^{|\xi|\pi/2}K_{\iota\xi}(|\xi|\epsilon)\ , \tag{A25}$$

where $K_{\iota\xi}$ is a modified Bessel function of imaginary order. From its definition we observe that $G_2(0,\epsilon)=0$ (the integrand is odd). It is simple to see (for example, by bounding the hyperbolic cosine by $\cosh u\ge1+u^2/2!+\cdots$) that, as $\xi\to0$,

$$\begin{aligned}|\mathrm{Im}G_2(\xi,\epsilon)|&\le2|\xi|\epsilon e^{|\xi|\pi/2}\int_0^{\infty}du\ e^{-|\xi|\epsilon(1+u^2/2)}\\&\le2|\xi|\epsilon e^{|\xi|(\pi/2-\epsilon)}\frac{1}{2}\left[\frac{\pi}{\epsilon|\xi|}\right]^{1/2}\end{aligned} \tag{A26}$$

which vanishes with $\xi\to0$, as it should in the hydrogenic limit. In fact, from (A16) we readily see (qualitatively) why the collision operator $\phi(\omega)$ has the "spike' seen in Fig. 1: For small, nonzero ω, ϕ rises from its hydrogenic value due to the extra contribution of G_2^2 in (A16). Later on, it will start decreasing due to inelasticity, of course.

Calculation of G_1

For G_1 we must first interchange our order of partial integration and contour deformation because the surface term from partial integration does not have a definite limit (we get $2\lim_{R\to\infty}\cos[\xi(\epsilon\sinh R-R)]$).

Then the contour deformation technique applied by Alder *et al.* [16] still gets no contribution from the sides, but now we have a double pole at $z=(0,\arccos(1/\epsilon))$. In contrast to our case, where we have $(\cosh u-1/\epsilon)$, Alder *et al.* had $(\cosh u+1/\epsilon)$ in the denominator and thus no singularity. The net result is that the residue from this double pole turns out to be 0 and it is as if we only had to change the sign of the exponent in the final expression. This point has been discussed by Klarsfeld [18]. For our purposes, it is clear that this difference is equivalent to replacing $e^{|\xi|\pi/2}$ by $e^{-|\xi|\pi/2}$ if we are interested in calculating the repulsive functions (as in the ion-dynamics check). So consider the same contour as before and the contour integral

$$\oint_C dz\frac{e^{\iota\xi(\epsilon\sinh z-z)}\left[1-\frac{\cosh z}{\epsilon}\right]}{(\cosh z-1/\epsilon)^2}=2\pi\iota b=0\ , \tag{A27}$$

where b is the residue. As far as the other line integrals

go, the vertical integrals again vanish (even more so now due to the denominator) and we obtain

$$G_1(\xi,\epsilon)=e^{|\xi|\pi/2}\int_{-\infty}^{\infty}du\frac{e^{-\iota\xi u}e^{-|\xi|\epsilon\cosh u}\left[1-\iota\dfrac{\sinh u}{\epsilon}\right]}{(\iota\sinh u-1/\epsilon)^2}\ . \tag{A28}$$

The integral may be evaluated by parts and we get the final formula for G_1:

$$G_1(\xi,\epsilon)=2\epsilon|\xi|e^{\pi|\xi|/2}\int_0^{\infty}\cos|\xi|u\,\cosh u e^{-|\xi|\epsilon\cosh u}du\ . \tag{A29}$$

The integral is, of course, the derivative of $-K_{\iota\xi}$.

Limiting behavior as $\xi\to 0$

Since for vanishing ξ the integrand in (A17) is an exact derivative $[\sinh u/(\cosh u-\epsilon^{-1})]$, integration gives $G_1(0,\epsilon)=2$. It can be easily shown that we get this result from (A29): $\cosh u=\sinh u+e^{-u}$, so

$$\int_0^{\infty}\cos|\xi|u\,\cosh u e^{-|\xi|\epsilon\cosh u}du$$

$$=\int_0^{\infty}\cos|\xi|ue^{-u}e^{-|\xi|\epsilon\cosh u}du$$

$$-\frac{1}{\epsilon|\xi|}\int_0^{\infty}\cos|\xi|u\,de^{-|\xi|\epsilon\cosh u}\ . \tag{A30}$$

When we take the limit $\xi\to 0$, the term involving e^{-u} will give 1, which will vanish when multiplied by the factor involving $|\xi|$ in front of the integral. The second term, when integrated by parts (in the surface term first $u\to\infty$, then $\xi\to 0$) gives a total contribution of

$$2\epsilon|\xi|\frac{1}{|\xi|\epsilon}\left[1-|\xi|\int_0^{\infty}\sin|\xi|ue^{-|\xi|\epsilon\cosh u}du\right]\ . \tag{A31}$$

The integral can be bound as before; i.e., drop the sine term, bound the cosh term by $1+u^2/2$, and evaluate the resulting Gaussian integral. The Gaussian integral will produce $|\xi|^{-1/2}$, which is "killed" by the $|\xi|$ multiplying the integral. The net result is that (A29) reproduces the correct $\xi=0$ result.

2. Direct terms

As far as the real parts so, we can split the real part of the direct term into four integrals, each of the type

$$\int_{-\infty}^{\infty}du_1\int_{-\infty}^{u_1}du_2 f(u_1)f(u_2)$$

$$=\tfrac{1}{2}\int_{-\infty}^{\infty}du_1\int_{-\infty}^{\infty}du_2 f(u_1)f(u_2) \tag{A32}$$

in the isolated line case $\xi_1=\xi=-\xi_2$. Hence the direct term in our case should reduce to one-half our interference term for $\xi_1=\xi=-\xi_2$. We get in this case from the above results

$$\mathrm{Re}G_d(\xi,-\xi,\epsilon)=\frac{2}{\epsilon^2}A(\xi,\epsilon)=\tfrac{1}{2}G_{\mathrm{int}}(\xi,-\xi,\epsilon)\ . \tag{A33}$$

3. Integration over ϵ

The ϵ integration gives

$$\int d\epsilon\,\epsilon G(\xi,-\xi,\epsilon)$$

$$=4e^{\pi|\xi|}\xi^2\int d\epsilon\,\epsilon\left[K'^2_{\iota\xi}(|\xi|\epsilon)+\frac{\epsilon^2-1}{\epsilon^2}K^2_{\iota\xi}(|\xi|\epsilon)\right]\ . \tag{A34}$$

With the transformation $x=|\xi|\epsilon$ we get

$$\int d\epsilon\,\epsilon G(\xi,-\xi,\epsilon)=4e^{\pi|\xi|}\int dx\left[\frac{x^2-\xi^2}{x}K^2_{\iota\xi}(x)+xK'^2_{\iota\xi}(x)\right] \tag{A35}$$

The integrand is just

$$\frac{d}{dx}xK_{\iota\xi}(x)K'_{\iota\xi}(x)=xK'^2_{\iota\xi}(x)+xK_{\iota\xi}(x)K''_{\iota\xi}(x)+K_{\iota\xi}(x)K'_{\iota\xi}(x) \tag{A36}$$

since

$$\frac{K_{\iota\xi}(x)}{x}[x^2K''_{\iota\xi}(x)+xK'_{\iota\xi}(x)-(x^2-\xi^2)K_{\iota\xi}(x)]=0\ , \tag{A37}$$

as may be verified by substituting the expressions for K and K' in the modified Bessel equation in brackets. With this we obtain

$$\phi_{\mathrm{int}}(\omega_1,-\omega_1)=\frac{8\pi n}{3}\left[\frac{e^2}{4\pi\epsilon_0\hbar}\right]^2\left[\frac{2}{\pi}\right]^{1/2}\left[\frac{m}{kT}\right]^{3/2}$$

$$\times\int_0^{\infty}dv\,ve^{-mv^2/2kT}e^{\pi|\xi|}|\xi|[\epsilon_{\max}K_{\iota\xi}(|\xi|\epsilon_{\max})|K'_{\iota\xi}(|\xi|\epsilon_{\max})|-\epsilon_{\min}K_{\iota\xi}(|\xi|\epsilon_{\min})|K'_{\iota\xi}(|\xi|\epsilon_{\min})|]\ . \tag{A38}$$

APPENDIX B: ASYMPTOTIC EXPRESSION FOR THE COLLISION OPERATOR

Defining the constant factor

$$q=\frac{4\pi n}{3}\left[\frac{e^2}{4\pi\epsilon_0\hbar}\right]^2\left[\frac{2}{\pi}\left[\frac{m}{kT}\right]^3\right]^{1/2}\ , \tag{B1}$$

the total collision operator is

$$\phi=q(\phi_1+\phi_2+\phi_s)\ , \tag{B2}$$

where

$$\phi_1=\int_0^{v_c}dv\,ve^{-mv^2/2kT}[a(\xi,\epsilon_{\max}(v))-a(\xi,1)]\ , \tag{B3}$$

$$\phi_2=\int_{v_c}^{\infty}dv\,ve^{-mv^2/2kT}[a(\xi,\epsilon_{\max}(v))-a(\xi,\epsilon_{\min}(v))] \tag{B4}$$

[compared to Eq. (13) there is a factor of q missing here.] ϕ_s is the strong-collision term, which in the hydrogenic case is

$$\phi_s = -\tfrac{1}{2}\int_{v_c}^{\infty} dv\,[1-(v_c/v)^2]ve^{-mv^2/2kT} . \tag{B5}$$

In the nonhydrogenic case, only Φ_s may be calculated, as in Appendix C. ϕ_1 and ϕ_2 are the contributions from $v<v_c$ and $v>v_c$, respectively. In the limit $\omega\to\infty$, ϕ_2 vanishes. ϕ_1 does not, however, vanish, but becomes

$$\begin{aligned}\phi_1(\omega\to\infty) &= -\frac{\pi}{\sqrt{3}}\int_0^{v_c} ve^{-mv^2/2kT}dv \\ &= -\frac{\pi}{\sqrt{3}}\frac{kT}{m}(1-e^{-mv^2/2kT}) .\end{aligned} \tag{B6}$$

observe that this is by no means negligible compared to the $\omega=0$ (hydrogenic) contribution.

The next question is for what value of ω can we set ϕ_1 equal to its asymptotic limit. Recalling the Poquerusse [20] approximation to the $a(\xi,\epsilon)$ function, valid for $\xi\geq 0.2$ and $\tau\leq 0.15$ (it is easy to show that $\tau\geq 0.15$ contributes negligibly in the large energy separation limit), with the adiabaticity parameter

$$\tau=\xi(\eta-\arctan(\eta)) , \tag{B7}$$

where

$$\eta=\sqrt{\epsilon^2-1} , \tag{B8}$$

$$\begin{aligned}a(\xi,\epsilon) = \frac{\pi}{\sqrt{3}} &+0.402\,15\xi^{-2/3}-1.7252\tau^{2/3}-0.0364\xi^{-4/3} \\ &+0.002\,03\xi^{-2}-0.861\,23\xi^{-2/3}\tau^{2/3}-1.941\tau^{4/3} \\ &+0.6744\xi^{-2/3}\tau^{4/3}+2.834\tau^2+0.040\,23\xi^{-4/3}\tau^{4/3}\end{aligned} \tag{B9}$$

(there is an obvious typo in the Poquerusse formulas, as the $m=2$, $n=1$ coefficient is given twice and the first one corresponds to $m=2$, $n=0$), we can keep only the first term provided that the remaining terms are much smaller. In fact we want to keep only the first term from the ϕ_1 contribution of $\rho_{\min}=0$ which gives (B6) and to be able to neglect the $\rho_{\max}$ contribution to ϕ_1 as well as the entire ϕ_2 term. It is most important to consider only the second and third terms in (B9), as all others are higher order in the smaller parameters $\tau^{2/3}$ and $\xi^{-2/3}$. The first requirement is satisfied if the second term is small compared to the first, say 0.1, and for this we need $\xi^{2/3}\geq 4 \Longrightarrow \xi\geq 8$ (not just 0.2). Thus for $\xi\geq 8$, ω must satisfy

$$\omega \geq \frac{32\pi\epsilon_0 m v_l^3}{e^2 Z_{\rm cm}} . \tag{B10}$$

With this bound for ξ, even for the $\rho_{\max}$ contribution, all terms are less than 3% of the first term, except for the third term (27%) and the seventh term (8.5%). Of course these are certainly overestimates as far as the total contribution to the width goes. For better accuracy, the (second) value used in (17) was obtained by demanding that the third term in (B9) be less than 0.1 for $v\geq 10^{-5}v_l$.

Also, in order for ϕ_2 to be safely neglected, we need $\tau(\rho_{\min}(v))\geq 0.15$, and this is satisfied with the last term in (17). The δ function means that ϕ_2 is nothing to worry about unless there is some significant part of the Maxwell-Boltzmann (MB) distribution for $v\geq v_c$. It was (rather generously) assumed that the MB distribution has "died" at $3\langle v\rangle$. Of course the above analysis aims at only safe estimates for $\omega_{\rm as}$.

APPENDIX C: ERROR ANALYSIS FOR THE COLLISION OPERATOR

We limit ourselves to a discussion *within* the framework of the impact approximation. We will use the semiclassical dipole collision operator for $\rho>\rho_{\min}$. The collisions with $\rho<\rho_{\min}$ produce the strong-collision contribution to Φ:

$$\Phi_{\rm str}=2\pi n\int_0^{\infty} dv\, vf(v)\int_0^{\rho_{\min}} d\rho\,\rho\{S_aS_b-1\} , \tag{C1}$$

where $\{\ \}$ is an angular average over the v angles and where S_a and S_b are the upper- and lower-level (diagonal) S-matrix elements. Clearly

$$0\geq\{\ \}=-\alpha\geq -2 . \tag{C2}$$

The total strong-collision contribution is then, in terms of the unknown α,

$$\begin{aligned}\Phi_{\rm str} = &-\pi n\alpha\left[\frac{2}{\pi}\right]^{1/2}\left[\frac{m}{kT}\right]^{3/2} \\ &\times\int_0^{\infty} dv\, v^3 e^{-mv^2/2kT}\rho_{\min}^2(v) .\end{aligned} \tag{C3}$$

The validity of the semiclassical approximation is guaranteed provided $\rho_{\min}$ is much larger than the maximum of the de Broglie wavelength $\hbar/mv$, the extent of the relevant atomic wave functions $n_a^2a_0/Z$ and the unitarity of the S matrix is not violated. We introduce a parameter b, such that for $\rho>b\hbar/mv$ the semiclassical picture is acceptable; i.e., the impact parameter is large enough compared to the de Broglie wavelength so that no problems arise on this front. We expect b to be between 1 and 10. There are then the following velocity scales.

(1) $v_0=b\hbar/m\rho_{\max}$. Collisions with $v<v_0$ have no semiclassical weak-collision contribution. No matter what the impact parameter, collisions cannot be treated semiclassically and as a result we can obtain a bound for their effect:

$$\begin{aligned}\Phi_{S0} &= -\pi n\alpha\left[\frac{2}{\pi}\right]^{1/2}\left[\frac{m}{kT}\right]^{3/2}\rho_{\max}^2\int_0^{v_0} v^3e^{-mv^2/2kT}dv \\ &= -\pi n\alpha\left[\frac{2m}{\pi kT}\right]^{1/2}\rho_{\max}^2\left[\frac{2kT}{m}(1-e^{-mv_0^2/2kT})\right. \\ &\qquad \left. -v_0^2e^{-mv_0^2/2kT}\right] .\end{aligned} \tag{C4}$$

(2) $v_1=\min(v_c, b\hbar Z/n_a^2a_0m)$. For collisions with $v<v_1$ the minimum impact parameter is $\rho_{\min}=b\hbar/mv$

and the strong-collision contribution from $v < v_1$ is

$$\Phi_{S1} = -\pi n \alpha \left[\frac{2}{\pi}\right]^{1/2} \left[\frac{m}{kT}\right]^{3/2} \left[\frac{b\hbar}{m}\right]^2 \int_{v_0}^{v_1} v e^{-mv^2/2kT} dv$$
$$= -\pi n \alpha \left[\frac{2m}{\pi kT}\right]^{1/2} \left[\frac{b\hbar}{m}\right]^2 (e^{-mv_0^2/2kT} - e^{-mv_1^2/2kT}) . \quad \text{(C5)}$$

Note that as long as $\rho_{\max} \gg \rho_{\min}$, $v_1 \gg v_0$.

(3) If $v_1 \neq v_c$, for $v > v_1$, the minimum impact parameter is determined by the relevant wave-function extent, $n_a^2 a_0/Z$, unless questions of violations of the unitarity of the S matrix arise. For electron broadening, in all cases considered except the C IV lines and with $b=1$, $\rho_{\min} = n_a^2 a_0/Z$ for $v > v_1 = b\hbar Z/n_a^2 a_0 m$; i.e., the semiclassical cutoff was always larger than the unitarity cutoff.

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