Dynamic screening effects in plasma line broadening

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The results of a kinetic theory of spectral-line broadening are applied to the calculation of Stark broadening for the Lyman-α line in the classical-path approximation. In the small-plasma-parameter limit, the width and shift operator reduces to an average binary electron-atom collision operator with screened interactions and dynamic correlations. The effects of screening, particularly the variation with frequency, are indicated for a simplified model and compared with the corresponding model without screening but with an impact-parameter cutoff in the collision integral. Comparison with the dynamically screened second-order (Born approximation) collision integral is also given.

I. INTRODUCTION

A kinetic theory formulation of spectral line shapes was proposed recently[1] in which the width and shift are determined by an exact effective atom-perturber binary collision operator. The approach is based on a formal kinetic theory designed to be "renormalized" in the sense that the actual interactions are screened by the correlations among particles. These effects have been included in most plasma line-broadening calculations by the introduction of cutoff parameters to restrict the range of the Coulomb interactions. Although the shielding should be substantially accounted for by such procedures, it is desirable to verify that this is the case and to provide the proper theoretical basis. The binary collision operator of Ref. 1 was calculated in the small-plasma-parameter limit, and with the screened interactions evaluated to lowest order in the atom-perturber coupling. The result is similar to the present unified theories,[2] but without the need for long-range cutoffs, since all atom-perturber interactions are shielded. One of the interactions is screened by the frequency-dependent dielectric function that produces full shielding at the line center, but no shielding in the wings. All other interactions appear shielded by the static Debye-Hückel pair correlation function.

The purpose here is to report a preliminary study of the importance of these screening effects in plasma broadening by studying the Lyman-α line in the dipole approximation, with no quenching and no lower state broadening. It is not our present objective to provide a refined line shape for the Lyman-α line, but rather to determine the relationship of the theoretically determined screening effects to those described by cutoff parameters, and additionally, to determine the accurate value of such parameters should cutoff procedures be desired for computational convenience. To put the calculation in proper context, therefore, it must be observed that removal of other commonly made approximations (e.g., dipole interaction, no time ordering, semiclassical scattering, ion-electron correlations) probably will generate additional quantitatively important corrections.[3] The calculation below is intended to parallel the present unified theory calculations[4] and makes all the same approximations with the exception that static and dynamic correlations are included; hence, we isolate only the effects of these correlations.

II. THEORY AND APPROXIMATIONS

A. Basic equations

The line profile for a neutral atom in a gas of ions and electrons is conveniently described by the function $I(\omega)$, defined by[3]

$$I(\omega) = \int_0^\infty d\epsilon\, P(\epsilon) J(\omega, \epsilon)\,, \tag{2.1}$$

where $P(\epsilon)$ is the electric microfield distribution function for the ions, and

$$J(\omega, \epsilon) = \pi^{-1}\, \mathrm{Im}\, \mathrm{Tr}_a \vec{d} \cdot [\Delta\omega - \mathcal{K}(\Delta\omega)]^{-1} f(a) \vec{d}\,. \tag{2.2}$$

The trace is taken over atomic states, and $\Delta\omega$ and $\mathcal{K}(\Delta\omega)$ are tetradic operators in the atomic subspace. Also $\vec{d}$ is the atomic dipole operator and $f(a)$ is the atomic density matrix. Equations (2.1) and (2.2) apply for dipole radiation and do not include Doppler effects. Furthermore, they are derived under the assumption that the ions are essentially static over the radiation time. These are reasonable approximations[3] for Lyman-α and will not be discussed further. The electron broadening is described by the operator $\mathcal{K}(\Delta\omega)$. In Ref.

1, this operator was formally expressed, without approximation, in terms of an average binary collision operator $T(a, 1; \Delta\omega)$;

$$\mathcal{K}(\Delta\omega) = -in\,\mathrm{Tr}_1 T(a, 1; \Delta\omega) f(a, 1) f^{-1}(a)\,, \qquad (2.3)$$

where the trace is taken over one-electron states, and $f(a, 1)$ is the reduced equilibrium density operator for the atom and one electron. The binary collision operator, $T(a, 1; \Delta\omega)$, satisfies a Lippmann-Schwinger–like equation with an effective atom-electron interaction and an average atom-electron propagator. These latter were evaluated in the small-plasma-parameter limit and to lowest order in the atom-electron coupling, with the result [see Eq. (4.9) of Ref. 1],

$$\mathcal{K}(\Delta\omega) = in \int d\vec{\mathrm{r}}_1\, d\vec{\mathrm{p}}_1\, L_1(a, 1) f(a) f(1) \times G(a, 1; \Delta\omega) \mathcal{L}(a, 1) f^{-1}(a)\,, \qquad (2.4)$$

with

$$G(a, 1; \Delta\omega) \equiv [\Delta\omega - L(1) + iH(1) - \mathcal{L}(a, 1)]^{-1} \qquad (2.5)$$

The classical limit has been taken for the electrons, and the notation is that of Ref. 1. Briefly, for an arbitrary operator θ,

$$\begin{aligned} &\Delta\omega\theta = (\omega - L(a, \epsilon))\,\theta\,, \\ &L(a, \epsilon)\theta = [H(a, \epsilon), \theta]\,, \\ &L_1(a, 1)\theta = [V(a, 1), \theta]\,, \\ &\mathcal{L}(a, 1)\theta = [\nu(a, 1), \theta]\,. \end{aligned} \qquad (2.6)$$

Here $V(a, 1)$ is the atom-electron potential. $H(a, \epsilon)$ is the atom Hamiltonian in the presence of the ion field

$$H(a, \epsilon) = H(a) - \vec{\epsilon} \cdot \vec{\mathrm{d}}\,. \qquad (2.7)$$

The potential $\nu(a, 1)$ is the screened atom-electron interaction

$$\nu(a, 1) = V(a, 1) + n \int d\vec{\mathrm{r}}_2 [g(r_{12}) - 1]\, V(a, 2), \qquad (2.8)$$

and $g(r)$ is the Debye-Hückel pair-correlation function. Also $L(1)$ and $H(1)$ are operators on electron functions, say $h(1)$, given by

$$\begin{aligned} &i\,L(1)h(1) \equiv (\vec{\mathrm{p}}_1/m) \cdot \vec{\nabla}_1 h(1); \\ &H(1)h(1) \equiv -f^{-1}(1)\, n \\ &\qquad \times \int d\vec{\mathrm{r}}_2\, d\vec{\mathrm{p}}_2 [\vec{\nabla}_1 V(1, 2)] \cdot \vec{\nabla}_{p_1} f(1) f(2) h(2). \end{aligned} \qquad (2.9)$$

The function $V(1, 2)$ is the Coulomb potential for particles 1 and 2, and $f(i)$ is the Maxwell-Boltzmann distribution for the ith electron.

The form of the result [Eq. (2.4)] may be simplified considerably as follows. First, $\mathcal{K}(\Delta\omega)$ may be rewritten

$$\mathcal{K}(\Delta\omega) = -in \int d\vec{\mathrm{r}}_1\, d\vec{\mathrm{p}}_1\, L_1(a, 1) f(a) f(1) \times G(a, 1; \Delta\omega) \Delta\omega f^{-1}(a)\,. \qquad (2.10)$$

Introducing the Fourier transform of $V(a, 1)$,

$$V(a, 1) = \int \frac{d\vec{\mathrm{k}}}{(2\pi)^3}\, e^{-i\vec{\mathrm{k}} \cdot \vec{\mathrm{r}}_1}\, \tilde{V}(a, k)\,.$$

Equation (2.10) becomes

$$\mathcal{K}(\Delta\omega) = -in \int \frac{d\vec{\mathrm{k}}}{(2\pi)^3}\, \tilde{L}_1(a, k) f(a) \times \tilde{G}(a, k; \Delta\omega) \Delta\omega f^{-1}(a)\,, \qquad (2.11)$$

where

$$\tilde{G}(a, k; \Delta\omega) \equiv \int d\vec{\mathrm{r}}_1\, d\vec{\mathrm{p}}_1 f(1)\, e^{-i\vec{\mathrm{k}} \cdot \vec{\mathrm{r}}_1} G(a, 1; \Delta\omega)\,. \qquad (2.12)$$

From the definition, (2.5), $G(a, 1; \Delta\omega)$ may be expressed as

$$G(a, 1; \Delta\omega) = [\Delta\omega - L(1) - \mathcal{L}(a, 1)]^{-1} \times [1 - iH(1) G(a, 1; \Delta\omega)]$$

Using the definition of $H(1)$ and substituting in Eq. (2.11) gives a form for $\mathcal{K}(\Delta\omega)$ in which all interactions are shielded:

$$\mathcal{K}(\Delta\omega) = -in \int \frac{d\vec{\mathrm{k}}}{(2\pi)^3}\, \tilde{\mathcal{L}}(a, k; \Delta\omega) f(a) \times \tilde{G}_0(a, k; \Delta\omega) \Delta\omega f^{-1}(a)\,, \qquad (2.13)$$

where

$$\begin{aligned} &\tilde{G}_0(a, k; \Delta\omega) \equiv \int d\vec{\mathrm{p}}_1\, d\vec{\mathrm{r}}_1\, e^{-i\vec{\mathrm{k}} \cdot \vec{\mathrm{r}}_1} f(p_1) \times [\Delta\omega - L(1) - \mathcal{L}(a, 1)]^{-1}\,, \\ &\tilde{\mathcal{L}}(a, k; \Delta\omega) \equiv \int \frac{d\vec{\mathrm{k}}'}{(2\pi)^3}\, \tilde{L}_1(a, k') \epsilon^{-1}(k', k; \Delta\omega)\,, \end{aligned} \qquad (2.14)$$

and $\epsilon(\vec{\mathrm{k}}, \vec{\mathrm{k}}'; \Delta\omega)$ is a generalized dielectric function satisfying the equation

$$\epsilon^{-1}(k, k'; \Delta\omega) = \delta(k - k') + \int \frac{d\vec{\mathrm{k}}''}{(2\pi)^3}\, I(k, k''; \Delta\omega) \times \left(\frac{k_D}{k''}\right)^2 \epsilon^{-1}(k'', k')\,,$$

$$I(k, k'; \Delta\omega) = \int d\vec{\mathrm{p}}_1\, d\vec{\mathrm{r}}_1 e^{-i\vec{\mathrm{k}} \cdot \vec{\mathrm{r}}_1} f(p_1) f(a) \times [\Delta\omega - L(1) - \mathcal{L}(a, 1)]^{-1}\, \frac{\vec{\mathrm{k}}' \cdot \vec{\mathrm{p}}_1}{m} \times e^{i\vec{\mathrm{k}}' \cdot \vec{\mathrm{r}}_1} f^{-1}(a).$$

The constant $k_D^2 \equiv 4\pi n e^2 \beta$ is the inverse Debye

length. Equation (2.13) is the main result for the width and shift operator in the small-plasma-parameter limit. All interactions are screened, so that divergences associated with the long-range nature of the Coulomb interaction have been removed. In addition, the presence of $\mathcal{L}(a,1)$ in the denominator of Eq. (2.13) assures that no strong collision cutoff procedure will be required for convergence.

The interaction $\mathcal{L}(a,\vec{k};\Delta\omega)$ is shielded by the dielectric function $\epsilon^{-1}(k,k';\Delta\omega)$. Since the other shielded interaction, $\mathcal{L}(a,1)$ in Eq. (2.13) was calculated only to lowest order in the atom-electron coupling (see Ref. 1 for details) the following discussion will limit $\mathcal{L}(a,\vec{k};\Delta\omega)$ also to lowest order in the atom-electron coupling. This is accomplished by setting $\mathcal{L}(a,1)$ equal to zero in the dielectric function. The latter then becomes diagonal in k so that the dynamically shielded interaction becomes

$$\mathcal{L}_0(a,k;\Delta\omega)=L_1(a,k)\epsilon^{-1}(k,\Delta\omega)\,, \tag{2.15}$$

$$\epsilon(k,\Delta\omega)=1-(k_D/k)^2 I_0(k;\Delta\omega)\,, \tag{2.16}$$

$$I_0(k,\Delta\omega)=\lim_{\alpha\to 0^+}\int d\vec{p}_1 f(p_1)\times\left(\Delta\omega-\frac{\vec{k}\cdot\vec{p}_1}{m}+i\alpha\right)^{-1}.$$

Here $\epsilon(k,\omega)$ is the usual dielectric function for an electron gas in the small-plasma-parameter limit, and is readily expressed in terms of the plasma dispersion function. It is interesting to note that, with the approximation (2.16), the $\Delta\omega=0$ limit of $\mathcal{L}(a,\vec{k};\Delta\omega)$ is simply the Fourier transform of the screened interaction $\mathcal{L}(a,1)$:

$$\mathcal{L}_0(a,k;\Delta\omega=0)=\tilde{\mathcal{L}}(a,k)\,.$$

Thus if the frequency dependence of $\mathcal{L}_0$ were neglected, the width and shift operator would be

$$\mathcal{K}(\Delta\omega)\to -in\int d\vec{p}_1\, d\vec{r}_1\,\mathcal{L}(a,1)f(a)f(1)\times[\Delta\omega-L(1)-\mathcal{L}(a,1)]^{-1}\times\mathcal{L}(a,1)\Delta\omega f^{-1}(a)\,. \tag{2.17}$$

This will be referred to as the statically screened result, and may be considered as the basis for the unified theory of Smith, Cooper, and Vidal. The latter is regained from Eq. (2.17) if the shielded interaction $\mathcal{L}(a,1)$ is replaced by the bare interaction $L_1(a,1)$ and the $\vec{r}_1$ integration cutoff outside a Debye sphere about the atom. In Sec. II it is found that the cutoff result differs noticeably from the statically screened result; interestingly, the error is in a direction such as to partially compensate for the difference between the dynamically and statically screened results.

B. Additional approximations

The expression above for the width and shift operator [Eqs. (2.13), (2.14), and (2.16)] is already in a tractable form; indeed $G_0(a,k;\Delta\omega)$ at $k=0$ may be expressed in terms of quantities already calculated in the unified theory.[4] However, to investigate the nature of the screening effects additional approximations will be made to further simplify the calculation while maintaining the essential features of the theory. Some of the approximations made are usual[4] in the description of the Lyman-α line and their validity will not be discussed. These are (i) no lower state broadening, (ii) dipole interaction between atom and electron, and (iii) no quenching. Approximation (i) allows $\mathcal{K}(\Delta\omega)$ to be represented as an ordinary operator in the atomic subspace rather than a tetradic. This is accomplished by the replacements

$$\Delta\omega\to\omega-H(a)+E_1-\vec{\epsilon}\cdot\vec{d}\,,\qquad L_1(a,1)\to V(a,1)\,, \tag{2.18}$$

where E_1 is the ground-state eigenvalue of $H(a)$. Also approximation (ii) means the atom-electron interaction is replaced by a dipole-monopole interaction

$$V(a,1)\to\vec{E}(1)\cdot\vec{d}\,, \tag{2.19}$$

where $\vec{E}(1)$ is the electric field of one electron.

The integral of the product of Fourier transforms in (2.13) may be written as the integral of the product of their inverse transforms,

$$\mathcal{K}(\Delta\omega)=-in\int d\vec{r}\,d\vec{p}\,\vec{E}(\vec{r},\Delta\omega)\cdot\vec{d}f(p)\times[\Delta\omega-L(1)-\vec{E}_s(1)\cdot\vec{d}]^{-1}\Delta\omega\,, \tag{2.20}$$

where

$$\vec{E}(\vec{r},\Delta\omega)\equiv\int\frac{d\vec{k}}{(2\pi)^3}e^{-i\vec{k}\cdot\vec{r}}\frac{\vec{E}(k)}{\epsilon(k,\Delta\omega)} \tag{2.21}$$

and $\vec{E}_s(1)$ is the statically shielded field: $\vec{E}_s(1)\equiv e(\vec{r}/r^2)(1+k_D r)\,e^{-k_D r}$. Further transformation is possible by factoring from $\vec{E}(r,\Delta\omega)$ its static value $\vec{E}_s(1)$,

$$\mathcal{K}(\Delta\omega)=-in\int d\vec{r}\,d\vec{p}f(p)W(\vec{r},\Delta\omega)\vec{E}_s(1)\cdot\vec{d}\times[\Delta\omega-L(1)-\vec{E}_s(1)\cdot\vec{d}]^{-1}\Delta\omega$$

where the weight function $W(\vec{r},\Delta\omega)$ contains all the dynamical shielding effects and is given by

$$W(\vec{r},\Delta\omega)\equiv\vec{r}\cdot\vec{E}(r,\Delta\omega)/\vec{r}\cdot\vec{E}_s(\vec{r})\,. \tag{2.22}$$

Transforming to a time representation gives

$$\mathcal{K}(\Delta\omega) = -n\int d\vec{r}\, d\vec{p} f(p) W(\vec{r}, \Delta\omega) \times \int dt\, \vec{E}_s(1)\cdot\vec{d}\exp\{[\Delta\omega - L(1) - \vec{E}_s\cdot\vec{d}]\, t\}\Delta\omega$$

$$= -in\int d\vec{r}\, d\vec{p} f(p) W(\vec{r}, \Delta\omega) \times \int_0^\infty dt \exp\{i[\Delta\omega - L(1)]\}\frac{d}{dt}[U(t) - 1]\Delta\omega\,. \tag{2.23}$$

Here $U(t)$ is the time-ordered exponential

$$U(t) \equiv T\exp\left(-i\int_0^t d\tau\, \vec{E}_s(1,\tau)\cdot\vec{d}(\tau)\right),$$

$$\vec{E}_s(1,t)\cdot\vec{d}(t) \equiv e^{-i[\Delta\omega - L(1)]t} \times \vec{E}_s(1)\cdot\vec{d}\, e^{i[\Delta\omega - L(1)]t}. \tag{2.24}$$

Two final approximations, also discussed in Ref. 4, are now introduced: the time dependence of the dipole operator $\vec{d}(t)$ is neglected, as is the effect of the time-ordering operator in $U(t)$. Equation (2.24) may then be written

$$\mathcal{K}(\Delta\omega) = in(\Delta\omega)\int_0^\infty dt\, e^{i\Delta\omega t}\int d\vec{r}\, d\vec{p} f(p) W\left(\vec{r} + \frac{\vec{p}}{m}t, \Delta\omega\right)\frac{d}{dt}\left\{\exp\left[-i\int_0^t d\tau\, E_s\left(\vec{r} + \frac{\vec{p}}{m}\tau\right)\cdot\vec{d}\right] - 1\right\}. \tag{2.25}$$

C. Atomic matrix elements

The Lyman-α line for hydrogen involves transitions from states of principal quantum number $n = 2$ to the ground state, so that $J(\omega, \epsilon)$ becomes

$$J(\omega, \epsilon) = \pi^{-1}\langle E_1|\vec{d}\circ[\Delta\omega - \mathcal{K}(\Delta\omega)]^{-1} f(a)\vec{d}\,|E_1\rangle, \tag{2.26}$$

where $|E_1\rangle$ is the ground state. Since $\Delta\omega$ is approximately diagonal in parabolic states, it is convenient to use the latter for representation of $[\Delta\omega - \mathcal{K}(\Delta\omega)]^{-1}$,

$$J(\omega, \epsilon) = \pi^{-1}\sum_{q,m}\sum_{q',m'}\langle E_1|\vec{d}|2, q, m\rangle\cdot\langle 2, q', m'|f(a)\vec{d}\,|E_1\rangle\langle 2, q, m|[\Delta\omega - \mathcal{K}(\Delta\omega)]^{-1}|2, q', m'\rangle, \tag{2.27}$$

where $|2, q, m\rangle$ denotes the parabolic state of principal quantum number 2 and q, m take on the values $-1, 0, 1$. To compute $J(\omega, \epsilon)$, therefore, the matrix elements of $\Delta\omega$ and $\mathcal{K}(\Delta\omega)$ with respect to parabolic states are required. As mentioned, $\Delta\omega$ is approximately diagonal, so that

$$\langle 2, q, m|\Delta\omega|2, q', m'\rangle = \delta_{q,q'}\delta_{m,m'}\Delta\omega(\beta, q)\,, \tag{2.28}$$

where $\Delta\omega(\beta, q)$ is the function

$$\Delta\omega(\beta, q) = \omega - (1/\hbar)(E_2 - E_1) - 3q(\hbar/me)\epsilon_0\beta\,,$$

E_1 and E_2 are the energies for the ground state and first excited state, respectively, β is the normalized ion field strength, $\beta \equiv \epsilon/\epsilon_0$, and $\epsilon_0 = (\frac{4}{3}\pi)^{2/3} en^{2/3}$. The calculation of the matrix elements of $\mathcal{K}(\Delta\omega)$ is discussed in the Appendix. The results are that $\mathcal{K}(\Delta\omega)$ is diagonal with respect to m, and the only off-diagonal elements with respect to q are those with $m = 0$:

$$\langle 2, 0, -1|\mathcal{K}|2, 0, -1\rangle = \langle 2, 0, 1|\mathcal{K}|2, 0, 1\rangle = F(\Delta\omega(\beta = 0, q = 0)),$$

$$\langle 2, 1, 0|\mathcal{K}|2, -1, 0\rangle = \tfrac{1}{2}\langle 2, -1, 0|\mathcal{K}|2, -1, 0\rangle = F(\Delta\omega(\beta, -1)), \tag{2.29}$$

$$\langle 2, -1, 0|\mathcal{K}|2, 1, 0\rangle = \tfrac{1}{2}\langle 2, 1, 0|\mathcal{K}|2, 1, 0\rangle = F(\Delta\omega(\beta, 1)),$$

and the function $F(\Delta\omega(\beta, q))$ is defined by

$$\tilde{\omega}_p^{-1} F(\Delta\omega_R(\beta, q)) = \tfrac{1}{3}i\pi[\Delta\omega_R(\beta, q)]^2 i(\Delta\omega_R(\beta, q))\,. \tag{2.30}$$

Here $\tilde{\omega}_p \equiv (8\pi ne^2/m)^{1/2}$ is $\sqrt{2}$ times the plasma frequency, and $\Delta\omega_R \equiv \Delta\omega(\beta, q)/\tilde{\omega}_p$. The function $i(\Delta\omega_R(\beta, q))$ is the analog of that introduced in the unified theory of Ref. 4, and is given by Eq. (A7) of the Appendix,

$$i(\omega) = -i8\pi n\omega^{-1}\int_0^\infty dt\, e^{i\omega t}\int_0^\infty dp\, p^2 f(p)\int_{-\infty}^\infty dz\int_0^\infty d\rho\,\rho W(r(t), \omega)\frac{d}{dt}\{\cos[3a_0 e^2 g(\rho, z, p, t)] - 1\}, \tag{2.31}$$

where $r(t) = \{\rho^2 + [z + (p/m)t]^2\}^{1/2}$, and

$$g(t) = (a^2 + b^2)^{1/2}, \quad a(t) = \int_0^t d\tau\frac{\rho(1 + k_D r(\tau))}{r^3(\tau)}e^{-k_D r(\tau)}, \quad b(t) = \int_0^t d\tau\left(z + \frac{p}{m}\tau\right)\frac{1 + k_D r(\tau)}{r^3(\tau)}e^{-k_D r(\tau)}. \tag{2.32}$$

Carrying out the time derivative in Eq. (2.31) and changing variables, $[z+(p/m)t]\to -z$, gives

$$i(\omega) = -8\pi nCi\omega^{-1}\int_0^\infty dt\, e^{i\omega t}\int_0^\infty dp\, p^2 f(p)\int_{-\infty}^\infty dz\int_0^\infty d\rho\,\rho\,\hat{r}\cdot\vec{E}(\vec{r},\omega)\left(\rho\frac{da(t)}{dt}+z\frac{db(t)}{dt}\right)\frac{\sin Cg}{g}, \tag{2.33}$$

where $C=3a_0e^2$ and the shielded field $\vec{E}(\vec{r},\omega)$ is given by Eq. (2.21).

The expression (2.33) is the principal result of this paper. For $\vec{E}(\vec{r},\omega)\to\vec{E}(\vec{r},\omega=0)$ it reduces to the impact approximation of Vidal, Cooper, and Smith,[4] except that the latter uses a Debye cutoff [as discussed following Eq. (2.17)] instead of the Debye-shielded field obtained here. More generally, the ω dependence of $\vec{E}(\vec{r},\omega)$ represents the dynamic screening of the electrons.

III. RESULTS

In this section the numerical calculations of Eq. (2.33) are reported for two cases of temperature and density. The first case is $T=12\,200$°K, $n=8.4\times10^{16}\,\mathrm{cm}^{-3}$, and a plasma parameter [$\Lambda\equiv(4\pi n\lambda_D^3)^{-1}$] of $\Lambda=0.052$. The second case is $T=25\,000$ °K, $n=3\times10^{18}\,\mathrm{cm}^{-3}$, and $\Lambda=0.106$. These conditions lie within the range of typical laboratory observations, in addition to meeting the requirement of small plasma parameter. For comparison, several approximations to Eq. (2.33) were also calculated.

A. Calculations using a Debye cutoff

The cutoff result, corresponding to the calculations of Ref. 4, is obtained by replacing the explicit shielding of fields by a cutoff of impact parameters outside the Debye sphere. This may be accomplished by setting $k_D=0$ everywhere in the integrand of (2.33) and replacing the upper limit of the ρ integration by a maximum impact parameter $\rho_{\max}$ giving

$$i_c(\omega) = -8\pi nCi\omega^{-1}\int_0^\infty dt\, e^{i\omega t}\int_0^\infty dp\, p^2 f(p)\int_{-\infty}^\infty dz\int_0^{\rho_{\max}} d\rho\,\rho\frac{dg_0}{dt}\sin(Cg_0), \tag{3.1}$$

where $g_0=(a_0^2+b_0^2)^{1/2}$ and

$$a_0=\frac{1}{\rho v}\left(\frac{z+vt}{r(t)}-\frac{z}{r(0)}\right);\quad b_0=\frac{1}{\rho v}\left(\frac{\rho}{r(t)}-\frac{\rho}{r(0)}\right). \tag{3.2}$$

In Ref. 4, a radial cutoff $[r_{\max}=(\rho_{\max}^2+z^2)^{1/2}]$ of 1.0 times the Debye length was used; others[5,6] have suggested cutoffs varying from 0.606 times the Debye length to 1.123 times the Debye length. Figure 1 shows $i_c(\omega)$ for cutoffs of 1.0 and 1.2. Since the large frequency limit of $i_c(\omega)$ is independent of the cutoff used, $i_c(\omega)$ in Fig. 1 has been normalized to its high-frequency limiting form. It is seen that the two cases differ in the low-frequency limit by about 10%. By requiring that the impact limits of this, $i_c(\omega)$, and the fully screened calculation, $i(\omega)$, be equal, it was determined that the optimum cutoff is approximately 1.15 times the Debye length.

B. Second-order calculations

Equation (2.33) has also been calculated to second order in the perturber-atom interaction[5,7] (Born approximation). In this limit $C\sin Cg\to C^2g$ and Eq. (2.33) becomes

$$i_2(\omega) = -8\pi nC^2i\omega^{-1}\int_0^\infty dt\, e^{i\omega t}\int_0^\infty dp\, p^2 f(p)\int_{-\infty}^\infty dz\int_0^\infty d\rho\,\rho\,\hat{r}\cdot\vec{E}(\vec{r},\omega)g\left(\rho\frac{da}{dt}+z\frac{db}{dt}\right). \tag{3.3}$$

With Eqs. (2.21) and (2.32), this may be rewritten

$$i_2(\omega)=\tfrac{1}{3}na_0^2e^2\int\frac{d\vec{k}}{(2\pi)^3}\frac{|\vec{E}(k)|^2}{\epsilon(k,\omega)}\lim_{\alpha\to0^+}\int d\vec{p}\,f(p)\left(\omega-\frac{\vec{k}\cdot\vec{p}}{m}+i\alpha\right)^{-1}, \tag{3.4}$$

which agrees with earlier results.[5,7] The $\vec{k}$ integration in Eq. (3.4) diverges at large k so that a cutoff at some $K_{\max}$ is required. The region of large k represents strong collisions with small impact parameters, for which the expansion in the perturber-atom interaction fails. Figure 2 shows $i_2(\omega)$ for several values of the strong collision impact parameter cutoff; it is seen that the behavior of $i_2(\omega)$ for $\omega>\omega_p$ is strongly dependent on this cutoff. Figure 3 shows a comparison of $i_2(\omega)$ with $i_c(\omega)$ and $i(\omega)$ where the strong collision cutoff used in $i_2(\omega)$ was chosen so that the $\omega\to0$ limit

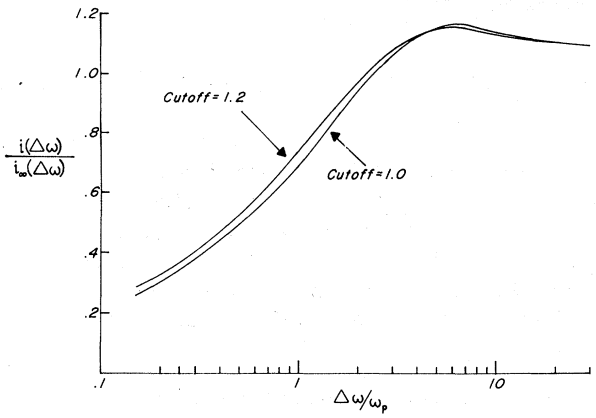

FIG. 1. $i_c(\Delta\omega)$ with cutoffs of $1.0\,\lambda_D$ and $1.2\,\lambda_D$, normalized to its infinite frequency asymptote for $T=12200\,^\circ\mathrm{K}$, $n=8.4\times10^{16}$.

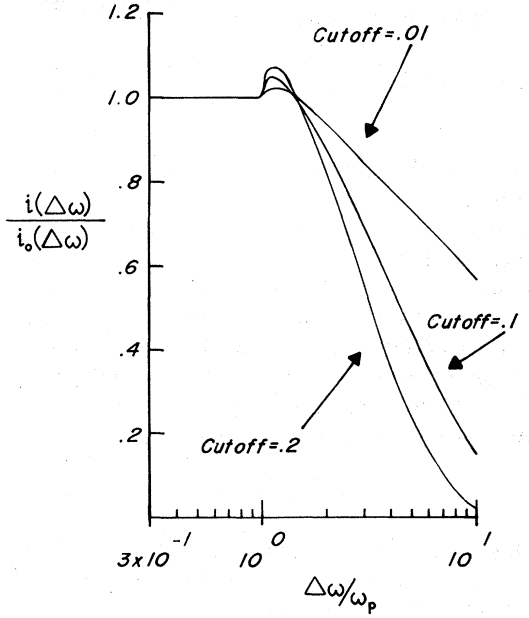

FIG. 2. $i_2(\Delta\omega)$, with several values of the strong collision cutoff, normalized to its zero-frequency asymptote. Note that $i_2(\Delta\omega)$ has no explicit temperature or density dependence.

of $i_2(\omega)$ agreed with that of $i(\omega)$. With this choice $i_2(\omega)$ and $i(\omega)$ are in excellent agreement out to several times the plasma frequency.

C. Static screening

To study the accuracy of the cutoff procedure in Sec. III A as well as to isolate the effects of dynamic screening, calculations were performed in which all interactions are taken to be statically screened [i.e., Eq. (2.17)]. This form is obtained from Eq. (2.33) by replacing $\vec{E}(r,\omega)$ with $\vec{E}_s(r)$, defined following Eq. (2.21), with the result,

$$i_s(\omega)=-8\pi nCi\omega^{-1}\int_0^\infty dt\, e^{i\omega t}\int_0^\infty dp\,p^2 f(p)\int_{-\infty}^{\infty} dz\int_0^\infty d\rho\,\rho\,\hat{r}\cdot\vec{E}_s(r)\left(\rho\frac{da}{dt}+z\frac{db}{dt}\right)\frac{\sin Cg}{g}\,. \tag{3.5}$$

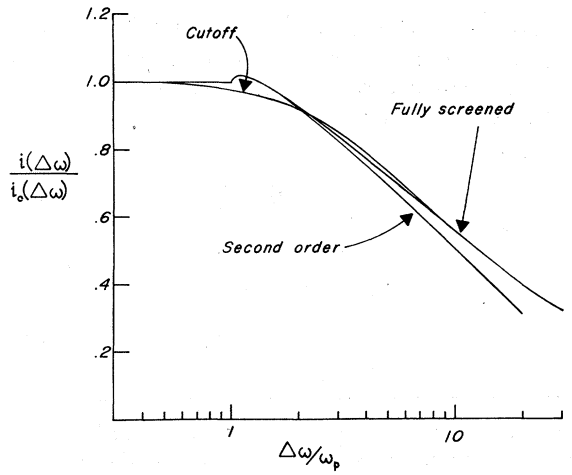

FIG. 3. $i_2(\Delta\omega)$ with strong collision cutoff chosen so that its $\Delta\omega\to0$ asymptote equals that of $i(\Delta\omega)$ for $T=12200\,^\circ\mathrm{K}$, $n=8.4\times10^{16}$. $i_c(\Delta\omega)$ and $i(\Delta\omega)$ are shown for comparison.

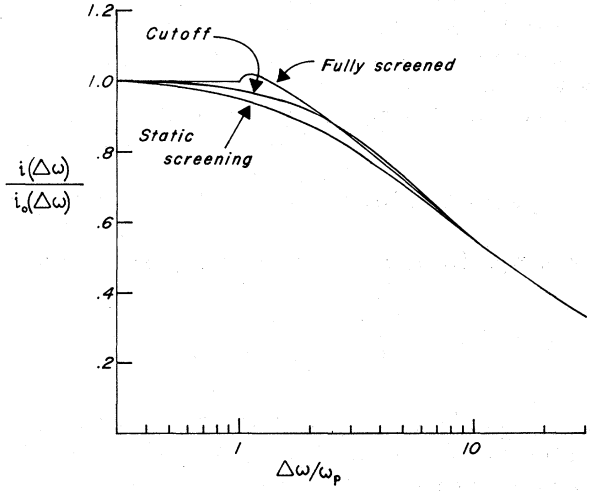

FIG. 4. Comparison of $i(\Delta\omega)$, $i_s(\Delta\omega)$ and $i_c(\Delta\omega)$ for $T=12200\,^\circ\mathrm{K}$, $n=8.4\times10^{16}$.

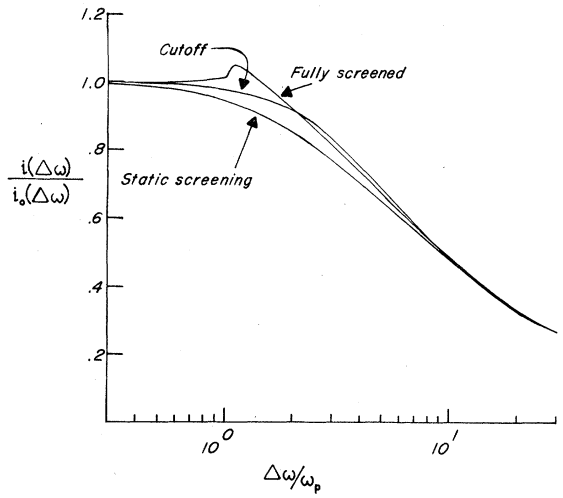

FIG. 5. Comparison of $i(\Delta\omega)$, $i_s(\Delta\omega)$, and $i_c(\Delta\omega)$ for $T=25000\,^{\circ}\mathrm{K}$, $n=3\times10^{18}$.

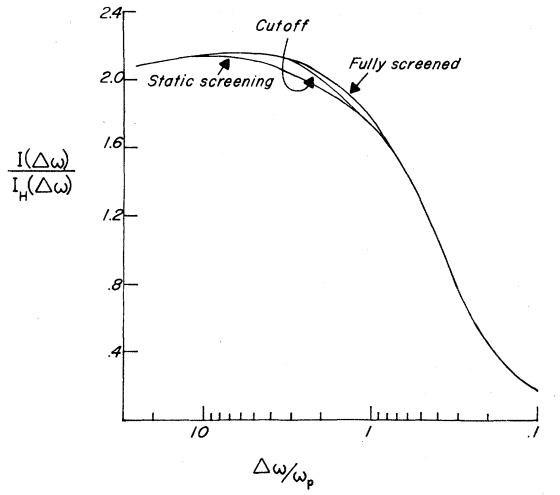

FIG. 7. Comparison of $I(\Delta\omega)$ (normalized to the $\Delta\omega^{-5/2}$ wing) for the cutoff, statically screened, and fully screened cases for $T=25000\,^{\circ}\mathrm{K}$, $n=3\times10^{18}$.

Figures 4 and 5 show a comparison of $i_s(\omega)$ and $i_c(\omega)$. The agreement at very small ω is essentially due to the choice of cutoff [see Sec. III B above]; also in the far wings there is agreement since there the strong collisions, for which shielding is less important, dominate. In the intermediate region, however, the cutoff Coulomb field overestimates the static Debye field for impact parameters of the order of the Debye length and $i_c(\omega)$ is greater than $i_s(\omega)$.

D. Full screening

Also included in Figs. 4 and 5 are the fully shielded results, $i(\omega)$, from Eq. (2.33). There is a small resonance near the plasma frequency, as expected from previous second-order calculations, due to the plasmon collective modes. The dynamical effects, in addition to this resonance, are clearly shown in the difference between the statically screened $i_s(\omega)$ and $i(\omega)$. The former lies below $i(\omega)$ for small ω because the dynamically shielded field is less than the Debye field for impact parameters of the order of the Debye length; at higher frequencies there is agreement, again because shielding is less important for the strong collisions which dominate in the wings. The fact that $i_c(\omega)$ agrees more closely with $i(\omega)$ than does $i_s(\omega)$ is a fortuitous consequence of the fact that both the cutoff Coulomb field and the dynamically shielded field are larger than the Debye field. Figures 6 and 7 show the corresponding line shapes, Eq. (2.1), normalized to the Holtsmark profile (the second-order model is not shown since it is qualitatively incorrect in the line wings). The ion microfield average has decreased the differences between $i(\omega)$, $i_s(\omega)$, and $i_c(\omega)$ to less than 5%.

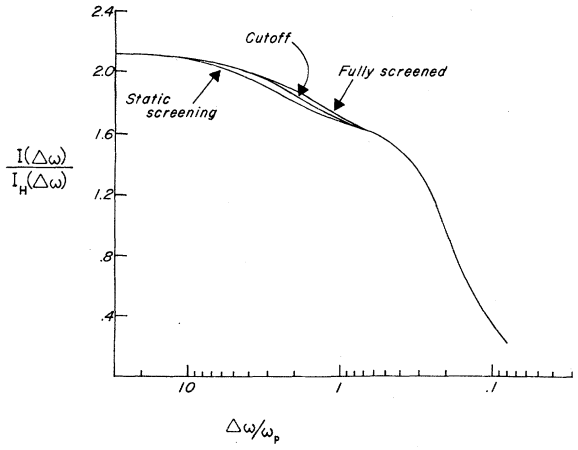

FIG. 6. Comparison of $I(\Delta\omega)$ (normalized to the $\Delta\omega^{-5/2}$ wing) for the cutoff, statically screened, and fully screened cases for $T=12200\,^{\circ}\mathrm{K}$, $n=8.4\times10^{16}$.

IV. CONCLUSION

The width and shift operator for electron broadening was evaluated to zeroth order in the plasma parameter, Λ, and with effective interactions to lowest order in the atom-electron coupling constant. Additional approximations to simplify computation were introduced paralleling the unified theory calculations of Ref. 4. The results indicate the following:

(i) The plasma parameter expansion of Ref. 1

gives a description of plasma line broadening free of any long-range Debye cutoff or strong collision cutoff, leading to impact limit behavior near line center, and Holtsmark wings; (ii) the effects of dynamic screening are noticeable in the range $0.1\omega_p \lesssim \omega \lesssim 10\omega_p$ (Figs. 4 and 5) although the maximum difference is only of the order of 10%; (iii) there is a small resonance at the plasma frequency (Figs. 4 and 5) as predicted by second-order theories which, however, is masked in the line profile (Figs. 6 and 7) by the ion microfield average; (iv) the low-frequency behavior, $\omega \lesssim 2\omega_p$, may be very accurately modeled by the phenomenological introduction of a suitable strong collision cutoff in the second-order theory (Fig. 3) although no simple form for such a cutoff is proposed; (v) the model using unshielded fields with a Debye cutoff is optimized with a radial cutoff at about 1.15 times the Debye length; nevertheless, the cutoff result differs from the statically screened result that it is intended to approximate over the region $0.2\omega_p \lesssim \omega \lesssim 10\omega_p$ (Figs. 4 and 5), although the differences are less than 5%; (vi) the form of screening is unimportant in the wings ($\omega \gtrsim 10\omega_p$); (vii) observations (iv) and (vi) suggest that screening may be less important for higher than second-order terms in an expansion of the collision operator in powers of the atom-electron interaction.[6] The unified theory of Capes and Voslamber,[8] in which screening (including dynamic effects) is included only to second order, is very likely quite adequate.

These conclusions are justified only for the Lyman-α line and for the small plasma parameters considered here. It is possible that the above differences may be amplified for larger plasma parameters or for higher series members.

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APPENDIX: MATRIX ELEMENTS OF $\mathcal{K}(\Delta\omega)$

Equation (2.27) requires inversion of the matrix $(\Delta\omega - \mathcal{K}(\Delta\omega))$ in a representation using the parabolic states. Since, as noted in Eq. (2.28) $\Delta\omega$ is diagonal in this representation, attention may be focused on the matrix elements of $\mathcal{K}(\Delta\omega)$. The parabolic states may be specified by the principal quantum number, n, the magnetic quantum number, m, and the quantum number $q = n_1 - n_2$, where n_1 and n_2 are the parabolic quantum numbers obeying the relation $n = n_1 + n_2 + |m| + 1$. In the no-quenching approximation, the z component of the dipole vector, $d_z = eZ$, is diagonal,

$$Z|n, q, m\rangle = \tfrac{3}{2} nqa_0 |nqm\rangle, \tag{A1}$$

where a_0 is the Bohr radius. This leads directly to the result (2.28) for the diagonal elements $\Delta\omega(\beta, q)$. For Lyman α, only the state of principal quantum number $n = 2$ is required for the matrix elements of $\mathcal{K}(\Delta\omega)$. Using Eq. (2.25) for $\mathcal{K}(\Delta\omega)$, we consider therefore,

$$\langle 2, q, m|\mathcal{K}(\Delta\omega)|2, q', m'\rangle = -in[\Delta\omega(\beta, q)] \int_0^\infty dt\, e^{i\Delta\omega(\beta,q)t} \int d\vec{r}\, d\vec{p} f(p) W\left(\vec{r} + \frac{\vec{p}}{m} t, \Delta\omega(\beta, q)\right)$$
$$\times \frac{d}{dt} \langle 2, q, m| \left\{ \exp\left[-i \int_0^t d\tau \vec{E}_s \left(\vec{r} + \frac{\vec{p}}{m} \tau \right) \cdot \vec{d} \right] - 1 \right\} |2, q', m'\rangle . \tag{A2}$$

It is convenient to introduce a cylindrical coordinate system for the $\vec{r}$ integration with axis along $\vec{p}$. The vector $\vec{r}$ then has components along $\vec{p}$ and in the radial direction $\vec{\rho}$ orthogonal to $\vec{p}$. The exponent in (A2) is therefore of the form

$$\int_0^t d\tau \vec{E}_s \left(\vec{r} + \frac{\vec{p}}{m} \tau \right) \cdot \vec{d} = \hat{\rho} \cdot \vec{d}\, a(r, p, t) + \hat{p} \cdot \vec{d}\, b(r, p, t), \tag{A3}$$

where a and b are scalar functions to be specified below. To facilitate the evaluation of the matrix element in (A2) we parallel the calculation of Ref. 4 by performing a rotation of the atomic axis such that the z direction is along $\vec{\rho}$, and the x direction along $\vec{p}$. Then (A2) may be simplified to

$$\langle 2, q, m|\mathcal{K}(\Delta\omega)|2, q', m\rangle = -in\Delta\omega(\beta, q) \int_0^\infty dt\, e^{i\Delta\omega(\beta,q)t} \int_0^\infty dp\, p^2 f(p) \int_{-\infty}^\infty dz \int_0^\infty d\rho\, \rho W(\rho, z, p, \Delta\omega(\beta, q))$$
$$\times \frac{d}{dt} \sum_{q'', m''} \{\exp[-i3q''a_0 e^2 g(\rho, z, p, t)] - 1\}$$
$$\times \int_0^{2\pi} d\phi \int d\Omega \langle 2, q, m|\mathfrak{D}|2, q'', m''\rangle \langle 2, q'', m''|\mathfrak{D}^{-1}|2, q', m'\rangle , \tag{A4}$$

where the function g is defined as

$$g=(a^2+b^2)^{1/2}\ , \tag{A5}$$

and $\mathfrak{D}$ is the atomic rotation operator. Also, use has been made of the fact that W is independent of the angular integration. The matrix elements of the rotation operators are most easily evaluated in a representation of spherical hydrogenic states, using the transformation

$$|n,q,m\rangle=\sum_{l,m}\langle nlm'|n_q m\rangle|nlm'\rangle,\ \langle nlm'|n_q m\rangle=\delta_{mm'}(-1)^{(1+m-q-n)/2}\ (2l+1)^{1/2}\begin{pmatrix}\frac{1}{2}(n-1) & \frac{1}{2}(n-1) & l\\ \frac{1}{2}(m-q) & \frac{1}{2}(m+q) & -m\end{pmatrix}\ ,$$

where l is the angular momentum quantum number and the parentheses denote a $3j$ symbol, and the identity

$$\int_0^{2\pi}d\phi\int d\Omega\ \mathfrak{D}^{(l)}_{m_1'm_1}\mathfrak{D}^{(l')*}_{m_2'm_2}=8\pi^2\delta_{m_1'm_2'}\delta_{m_1m_2}\delta_{l,l'}(2l+1)^{-1}\ .$$

With these results Eq. (A4) becomes

$$\langle 2,q,m|\mathcal{K}(\Delta\omega)|2,q',m'\rangle=i\pi\tilde{\omega}_p\delta_{m,m'}[\Delta\omega_R(\beta,q)]^2\,i(\Delta\omega_R)$$
$$\times\left[(-1)^{1+m-(1/2)(q+q')}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & 1\\ \frac{1}{2}(m-q) & \frac{1}{2}(m+q) & -m\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & 1\\ \frac{1}{2}(m-q') & \frac{1}{2}(m+q') & -m\end{pmatrix}+\tfrac{1}{2}\delta_{m,0}\right]. \tag{A6}$$

Here the function $i(\omega)$ is the analog of that introduced in Ref. 4, and is given by

$$i(\omega)\equiv-i\omega^{-1}8\pi n\int_0^\infty dt\ e^{i\omega t}\int_0^\infty dp\,p^2f(p)\int_{-\infty}^\infty dz\int d\rho\,\rho\,W(r(t),\omega)\frac{d}{dt}\{\cos[3a_0e^2g(\rho,z,p,t)]-1\}, \tag{A7}$$

where $r(\tau)\equiv[\rho^2+(v\tau+z)^2]^{1/2}$. Also $\Delta\omega_R\equiv\Delta\omega/\tilde{\omega}_p$, where $\tilde{\omega}_p^2=8\pi ne^2/m$. Evaluation of the 3-$j$ symbols in (A6) gives the results (2.29), (2.30), and (2.31) of Sec. II.

The function $g(\rho,z,v,t)$ is determined from the functions a and b through Eq. (A5) and

$$a=\int_0^t d\tau\frac{\rho(1+k_Dr(\tau))e^{-k_Dr(\tau)}}{r^3(\tau)},\quad b=\int_0^t d\,\frac{(v\tau+z)(1+k_Dr(\tau))e^{-k_Dr(\tau)}}{r^3(\tau)}\ . \tag{A8}$$

Finally, the shielded field is given by

$$\hat{r}\cdot\vec{E}(r,\omega)=\alpha(r,\omega)+i\beta(r,\omega), \tag{A9}$$

with

$$\alpha(r,\Delta\omega)=\frac{2}{x\pi}\int_0^\infty\frac{dz}{z}\ \frac{\sqrt{\pi}\,(z^3/\omega_R^2)e^{-z^2}h(\omega_p x/z)}{[1+(z^2/\omega_R^2)(1-\phi(z))]^2+\pi(z^3/\omega_R^2)^2e^{-2z^2}}\ ,$$
$$\beta(r,\Delta\omega)=\frac{2}{x\pi}\int_0^\infty\frac{dz}{z}\ \frac{[1+(z^2/\omega_R^2)(1-\phi(z))]h(\omega_R x/z)}{[1+(z^2/\omega_R^2)(1-\phi(z))]^2+\pi(z^3/\omega_R^2)^2e^{-2z^2}}\ . \tag{A10}$$

Here $x=k_Dr=k_D(\rho^2+z^2)^{1/2}$, $\phi(z)$ is Dawson's integral

$$\phi(z)=2ze^{-z^2}\int_0^z dy\ e^{y^2}\ , \tag{A11}$$

and the function $h(y)$ is

$$h(y)=\sin y-y\cos y. \tag{A12}$$

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