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Ion Motion in Plasma Line Broadening*

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A recently developed method to study ion-motion effects on plasma line broadening in the dipole approximation is extended to the general interaction. Coupling-constant and binary-collision expansions are obtained for the "width and shift" operator. This operator is investigated for a model system to show the limits of the static-ion approximation.

I. INTRODUCTION

The spectral line shapes for atoms emitting radiation in a plasma are determined by the interaction of the atom with all the components of the plasma.¹ For a large portion of the line profile, the relatively heavy ions may be treated as static and their effects accounted for by the introduction of an ion microfield.^{1,2} It was shown recently³ that the ion microfield function can be introduced formally exactly, thus explicitly accounting for the large static-field contributions without the usual static-ion assumptions. The dynamics of the perturbers in interaction with the atom was treated in a collisional approximation by second-order perturbation theory. The resulting expression for the line shape is formally similar to earlier work,^{2,4} with generalization to include ion motion. Another important advantage is that ion-electron interactions need not be treated in an indirect manner.⁵

Here, this method of investigating the role of ion dynamics will be continued and extended. Reference 3 was limited to the case of dipole inter-

action between the atom and perturber. This is extended in Sec. II to the general case in which all charges interact through a Coulomb potential. The width and shift operator is determined to second order in the plasma-atom interaction. Since the Coulomb interaction is large for small distances this result cannot be correct for close, or strong collisions. To account for these, a binary-collision expansion⁶ of the width and shift operator is given in Sec. III. The first term in the expansion is essentially the impact approximation^{1,7} including ion-motion effects. In the last section, a random-phase approximation is used to determine how close to the line center a static-ion theory should be used. The region in which ion motion is important is found to be an order of magnitude larger than usually estimated. However, it is indicated that this result is not realistic due to an unjustified extension of the electron strong-collision cutoff procedure to the ions. The cutoff for the electrons has been studied by Shen and Cooper⁸ by an evaluation of the atom-electron t matrix. The starting point for a corresponding study of the ions is provided by the results of

Sec. III. Nevertheless, it is expected that the qualitative aspects of this model are correct.

An important investigation of the ion dynamics has been carried out by Kogan,⁹ who considered an ideal gas of electrons and ions in dipole (and quadrupole) interaction with the atom. First-order corrections to the static microfield contribution, which for his model is the Holtzmark profile, were calculated. Since his calculation, it has become clear that correlations due to interactions have an important effect on the microfield itself, as well as the dynamics. Thus, the model considered by Kogan is not realistic, although it serves well to describe the qualitative aspects of the dynamics with respect to the Holtzmark profile, and reconsideration of Kogan's work with more careful numerical evaluation could be instructive. The result of Sec. III below is exact for the model considered by Kogan. The most complete realistic description of the entire line profile has been given recently by Smith, Cooper, and Vidal.¹⁰ They assume static ions, but claim to describe the entire line shape outside the region of breakdown of this assumption. It is shown below that the result of Sec. III obtained here reduces to their "unified line-shape approximation" if contributions from ion motion are neglected. Contact with the impact and one-electron theories is thus made through Ref. 10.

II. GENERAL THEORY

The essential details of the line shape are contained in the function $I(w)$,¹

$$I(w) = \text{Re}[(\pi)^{-1} \int_0^\infty dt e^{iwt} \text{Tr} \rho_a \rho_p \vec{d} \cdot \vec{d}(t)] \quad (2.1)$$

where Tr indicates a trace over a complete set of states for the atom and plasma, ρ_a and ρ_p are, respectively, density matrices for the atom and plasma, and $\vec{d}(t)$ is the Heisenberg operator, $\vec{d}(t) = e^{iHt} \vec{d} e^{-iHt}$ (in units such that $\hbar = 1$). Here, \vec{d} is the atomic dipole operator and the Hamiltonian H is of the form

$$H = H_a + H_p + \lambda H_I \quad (2.2)$$

H_a and H_p are the free-atom and plasma Hamiltonians, respectively, and H_I is their interaction (a coupling constant λ is introduced for later use). The Liouville operator for the system may be defined by

$$Lf = i[H, f] \quad (2.3)$$

where f is an arbitrary operator on the Hilbert space of the system. It is readily shown that (2.1) may be written

$$I(w) = -(\pi)^{-1} \text{Im} \text{Tr} \rho_a \rho_p \vec{d} \cdot R(w) \vec{d} \quad (2.4)$$

$$R(w) = (w - iL)^{-1} \quad (2.4)$$

$R(w)$ is the resolvent operator for L . The trace in (2.4) may be performed in two stages by choosing the complete set of states to be formed from the direct product of sets complete in the atomic and plasma subsystems. Since ρ_p commutes with \vec{d} , the line-shape function may be written

$$I(w) = -(\pi)^{-1} \text{Im} \text{Tr} \rho_a \vec{d} \cdot \langle R(w) \rangle \vec{d} \quad (2.5)$$

where the brackets $\langle \rangle$ indicate an ensemble average over the plasma

$$\langle f \rangle = \text{Tr} \rho_p f \quad .$$

The line shape can therefore be calculated from the plasma-averaged resolvent. Before proceeding to the case of interest here we note for future reference that inside the ion plasma frequency, i. e., very close to the line center, there is no large static contribution to $\langle R(w) \rangle$ since these frequencies correspond to times sufficiently large for all charges to move. In this region, it is useful to define an operator $M(w)$ by

$$\langle R(w) \rangle = [w - iL_a - iM(w)]^{-1}, \quad L_a f = i[H_a, f] \quad (2.6)$$

Equation (2.6) may be solved algebraically for $M(w)$, using familiar properties of the resolvent operator. A straightforward expansion to second order in the coupling constant λ leads to results obtained previously in this way for electron broadening² with the obvious changes to include corresponding ion terms. The above is essentially the method proposed by Fano.¹¹ Expansion in parameters other than the coupling constant are possible (such as considered in Sec. III).

The principal interest here will be in describing the line shape for frequencies large enough for static-ion effects to dominate. One of the purposes here is to provide a formalism capable of defining this region more accurately. In principle, (2.6) may be used over the entire line profile. However, the complexity of $M(w)$ restricts its practicality to cases for which finite-order perturbation theory in some parameter is meaningful. In particular, it is possible to show the static-ion contributions to $M(w)$ may not be obtained by finite-order perturbation theory. Therefore, a better starting point is the static-ion approximation, in which the ions are assumed not to move at all and their static-field contribution is calculated from an average ion microfield function. The electrons are then treated in a manner corresponding to (2.6) for the electrons alone. A principal result of Ref. 3 was to show that it is possible to introduce the static-ion microfield function without the static-ion assump-

tions. Therefore, in this formulation, the supposed dominant static-ion contribution is accounted for while including whatever ion motion still contributes. This is then the proper starting point for finite-order perturbation approximations when static-ion effects are important.

Reference 3 was restricted to the case in which the atom and plasma interact via a dipole potential. This interaction is adequate only for perturbers that remain sufficiently far from the atom. In the following, the results of Ref. 3 are extended to the general interaction in which the perturbers interact with each atomic component by means of a Coulomb potential. Since the ion field now does not occur in the Hamiltonian, the introduction of an average ion microfield distribution function must be considered somewhat artificial. Nevertheless, it can be seen that the dominant static contribution comes from those ions sufficiently far from the atom as to allow the dipole approximation. Indeed, inside the region of breakdown of the dipole approximation even slight motion changes the value of the interaction potential significantly, whereas the same motion for more distant ions yields little change. This indicates that the ion microfield function gives the dominant static contribution, even when the interaction is not dipole. These comments are not made to justify any approximation but rather to motivate the formulation below which follows as an identity from (2. 1).

Corresponding to the decomposition of the Hamiltonian (2. 2) the Liouville operator is written

$$L = L_a + L_p + \lambda L_I, \quad (2. 7)$$

in an obvious notation. The interaction operator L_I may be further written

$$L_I = L_{ia} + L_{ea},$$

corresponding to the ion-atom and electron-atom interactions

$$V_{ia} = e^2 \sum_{\alpha=1}^{N/2} \left(\frac{1}{|r_n - q_{\alpha i}|} - \frac{1}{|r_e - q_{\alpha i}|} \right), \quad (2. 8)$$

$$V_{ea} = e^2 \sum_{\alpha=1}^{N/2} \left(\frac{1}{|r_e - q_{\alpha e}|} - \frac{1}{|r_n - q_{\alpha e}|} \right).$$

The quantities r_n and r_e are the positions of the atomic nucleus and atomic electron; $q_{\alpha i}$ and $q_{\alpha e}$ denote the positions of the α th ion and electron, respectively. The system has been chosen to be charge neutral. Equation (2. 5) shows the main task is to calculate $\langle R(w) \rangle$. This will be done in a manner paralleling Ref. 3, as follows. Let $L_{ia}(E)$ be the Liouville operator for the atom-ion interaction if the dipole approximation were used,

$$L_{ia}(E_i)f = i[\vec{E}_i \cdot \vec{d}, f], \quad \vec{E}_i = \sum_{\alpha=i}^{N/2} e \frac{q_{\alpha i}}{|q_{\alpha i}|^3},$$

i. e., \vec{E}_i is the electric field due to the ions. Define an operator \mathcal{H} in the atomic subsystem (independent of plasma coordinates) by

$$\langle R(w) \rangle = \langle [w - iL_a - i\lambda L_{ia}(E_i) - i\mathcal{H}(w)]^{-1} \rangle. \quad (2. 9)$$

It is important to realize that (2. 9) is a definition of \mathcal{H} , and although the dipole interaction term $L_{ia}(E_i)$ appears on the right-hand side, no approximation is implied. For this reason, as mentioned above, the introduction of $L_{ia}(E_i)$ is artificial in the sense that its contribution to the average in (2. 9) must be compensated for by terms in \mathcal{H} . The argument of $\mathcal{H}(w)$ anticipates the fact that it depends on w .

The reason for such a peculiar definition is, as shown by the corresponding case considered in Ref. 3, that the average microfield function may be introduced without assumption,

$$\begin{aligned} & \langle [w - iL_a - i\lambda L_{ia}(E_i) - i\mathcal{H}(w)]^{-1} \rangle \\ &= \int d^3 \mathcal{E} \langle \delta(\vec{\mathcal{E}} - \vec{E}_i) [w - iL_a - i\lambda L_{ia}(\vec{E}_i) - i\mathcal{H}(w)]^{-1} \rangle \\ &= \int d^3 \mathcal{E} \langle \delta(\vec{\mathcal{E}} - \vec{E}_i) [w - iL_a - i\lambda L_{ia}(\mathcal{E}) - i\mathcal{H}(w)]^{-1} \rangle \\ &= \int d^3 \mathcal{E} \langle \delta(\vec{\mathcal{E}} - \vec{E}_i) [w - iL_a - i\lambda L_{ia}(\mathcal{E}) - i\mathcal{H}(w)]^{-1} \rangle \\ \text{or } I(w) &= \int d^3 \mathcal{E} Q(\vec{\mathcal{E}}) J(w, \vec{\mathcal{E}}), \end{aligned}$$

$$Q(\vec{\mathcal{E}}) = \langle \delta(\vec{\mathcal{E}} - \vec{E}_i) \rangle, \quad (2. 10)$$

$$J(w, \vec{\mathcal{E}}) = (\pi)^{-1} \text{Im Tr} \rho_a \vec{d} \cdot [w - iL_a - i\lambda L_{ia}(\mathcal{E}) - \mathcal{H}(w)]^{-1} \vec{d}.$$

The important step above is the replacement of $L_{ia}(\vec{E}_i)$ by $L_{ia}(\mathcal{E})$ after the δ function is introduced, which is possible only if \vec{E}_i commutes with everything in the denominator. This latter point is motivation for definition (2. 9). We emphasize that (2. 10) is an exact consequence of (2. 1) in which no dipole interaction for any of the perturbers is implied.

The operator $\mathcal{H}(w)$ must be determined from its definition, (2. 9). This is not practically possible in all generality. However, since the large static-ion contributions have already been summed in the microfield function, we may expect finite-order perturbation theory to be meaningful for $\mathcal{H}(w)$ [whereas it is not for $M(w)$ in (2. 6)]. If it is assumed that the dynamical effect of the ions and electrons on the atom is weak, $\mathcal{H}(w)$ may be expanded in the coupling constant λ . For close encounters between perturbers and the atom this assumption is not valid, and the case in which contributions from such collisions are important is treated in Sec. III. A straightforward

expansion of the left- and right-hand sides of (2.9) determines $\mathfrak{K}(w)$ to second order-in λ as

$$\mathfrak{K}(w) = \lambda^2 \left[\langle L_I K L_I \rangle - \langle L_{i_a}(\vec{E}_i) K_a L_{i_a}(\vec{E}_i) \rangle \right], \quad (2.11)$$

$$K = (w - iL_a - iL_p)^{-1}, \quad K_a = (w - iL_a)^{-1}.$$

This differs from Eq. (2.22) of Ref. 3 in that L_I here is defined in terms of the exact interaction (2.8) whereas the other holds only in the dipole approximation. Following the analysis of Ref. 3 it is found that the matrix representation of \mathfrak{K} (in terms of eigenvectors of H_a) is

$$\langle \mu | \mathfrak{K} f | \nu \rangle = \sum_{\mu', \nu'} \mathfrak{K}_{\mu\nu, \mu'\nu'} f_{\mu'\nu'},$$

where

$$\begin{aligned} \mathfrak{K}_{\mu\nu, \mu'\nu'}(w) &= \lambda^2 \left[\left(G_{\mu\mu', \nu\nu'}^R(\Delta w_{\nu\mu'}) - \frac{1}{3} \vec{d}_{\mu\mu'} \cdot \vec{d}_{\nu\nu'} \frac{\langle E_i^2 \rangle}{\Delta w_{\nu\mu'}} \right) \right. \\ &+ \left. \left(G_{\mu\mu', \nu\nu'}^A(-\Delta w_{\nu'\mu}) - \frac{1}{3} \vec{d}_{\mu\mu'} \cdot \vec{d}_{\nu\nu'} \frac{\langle E_i^2 \rangle}{\Delta w_{\nu'\mu}} \right) \right] \\ &- \lambda^2 \sum_{\nu''} \left[\delta_{\nu\nu''} \left(G_{\mu\nu'', \nu''\mu'}^R(\Delta w_{\nu\nu''}) - \frac{1}{3} \vec{d}_{\mu\nu''} \cdot \vec{d}_{\nu''\mu'} \frac{\langle E_i^2 \rangle}{\Delta w_{\nu\nu''}} \right) \right. \\ &\cdot \vec{d}_{\nu''\nu'} \frac{\langle E_i^2 \rangle}{\Delta w_{\nu\nu''}} + \delta_{\mu\mu'} \left(G_{\nu'\nu'', \nu''\nu}^A(-\Delta w_{\nu'\nu''}) \right. \\ &\left. \left. - \frac{1}{3} \vec{d}_{\nu'\nu''} \cdot \vec{d}_{\nu''\nu} \frac{\langle E_i^2 \rangle}{\Delta w_{\nu'\nu''}} \right) \right]. \quad (2.12) \end{aligned}$$

Here $\Delta w_{\mu\nu}$ is the difference $w - (\mathcal{E}_\mu - \mathcal{E}_\nu)$ and $\mathcal{E}_\mu, \mathcal{E}_\nu$ are eigenvalues of H_a . The functions $G^R(w)$ and $G^A(w)$ are defined by

$$G_{\mu\nu, \mu'\nu'}^A(w) = [G_{\nu'\mu', \nu\mu}^R(w)]^*,$$

$G_{\mu\nu, \mu'\nu'}^R$

$$\begin{aligned} &= 4(\pi)^{-1} \left(n(\omega) \int_0^\infty \frac{dk}{k} \frac{\text{Im}\epsilon(k, \omega)}{|\epsilon(k, \omega)|^2} A_{\mu\nu, \mu'\nu'}(k) \right. \\ &+ \frac{i}{\pi} P \int_{-\infty}^\infty d\omega' \frac{n(\omega')}{\omega - \omega'} \\ &\left. \times \int_0^\infty \frac{dk}{k} \frac{\text{Im}\mathcal{E}(k, \omega')}{|\mathcal{E}(k, \omega)|^2} A_{\mu\nu, \mu'\nu'}(k) \right). \quad (2.13) \end{aligned}$$

$\epsilon(\vec{k}, w)$ is the exact dielectric constant for the two-component plasma,¹² $n(\omega) = (e^{\beta\omega} - 1)^{-1}$, and

$$\begin{aligned} A_{\mu\nu, \mu'\nu'}(k) &= 8e^2 \int \int d^3R d^3R' \\ &\times \phi_\mu^*(R) \phi_\nu(R) \phi_{\mu'}^*(R') \phi_{\nu'}(R') \left(\frac{\sin k |R - R'|}{|R - R'|} \right. \\ &\left. - \frac{\sin k |R|}{|R|} - \frac{\sin k |R'|}{|R'|} + k \right). \quad (2.14) \end{aligned}$$

The atomic wave functions in (2.14) are in the relative coordinate system. Expansion of the bracketed term in (2.14) to lowest nonvanishing order in k yields, in conjunction with (2.13), the dipole approximation results of Ref. 3. Further investigation of these results is provided in Sec. IV.

III. BINARY-COLLISION EXPANSION

The expression for $\mathfrak{K}(w)$ given by (2.11) is essentially a Born approximation in the atom-perturber scattering. This description breaks down for close collisions and to account for these, an expansion in two-body t matrices⁶ will be obtained. These two-body t matrices describe the exact scattering of a perturber and atom in the presence of all other perturbers. Collisions in which more than one perturber is involved with the atom are accounted for by terms containing products of two-body t matrices. If the system being considered were a simple one-component gas interacting by means of short-ranged forces, the two particle t matrices would be proportional to the scattering length. For particles without internal degrees of freedom this leads to an expansion in the density. Here, the interaction is long ranged and one of the particles involved in the scattering has internal structure, and this interpretation of the binary-collision expansion must be modified as discussed below.

The operator $\mathfrak{K}(w)$ must again be determined from its definition [Eq. (2.9)]. The left-hand side of (2.9) is rewritten in a convenient form by observing that the resolvent operator satisfies

$$R(w) = K + iK L_I R, \quad (3.1)$$

where K is defined following (2.11). Define a T operator by

$$TK = -iL_I R. \quad (3.2)$$

Use of (3.2) in (3.1) shows

$$T = -iL_I + L_I K T. \quad (3.3)$$

Then, in terms of T , we obtain

$$\langle R(w) \rangle = \langle K(w) \rangle - \langle K(w) T(w) K(w) \rangle$$

or $\langle R(w) \rangle = K_a(w) - K_a(w) \langle T(w) \rangle K_a(w)$. (3.4)

Use has been made of the fact that $\langle L_p K \rangle = 0$.

Thus, $\langle R(w) \rangle$ may be determined from $\langle T(w) \rangle$.

The two-body operators are defined by

$$t_\alpha = -iL_\alpha + iL_\alpha K t_\alpha, \quad (3.5)$$

where $L_\alpha f = i[V_\alpha, f]$, V_α is the interaction potential between the α th perturber and the atom. Since one of the particles in the two-body scatterings considered is always the atom, the single param-

eter α is used to label the perturber involved. The T operator may be expressed in terms of the t_α as follows¹³: Let \bar{t}_α be defined by

$$\bar{t}_\alpha = -iL_\alpha + TKiL_\alpha,$$

$$\text{so } T(w) = \sum_{\alpha=1}^N \bar{t}_\alpha(w). \quad (3.6)$$

But

$$-\bar{t}_\alpha + \bar{t}_\alpha K t_\alpha = (TK - 1)iL_\alpha(Kt_\alpha - 1) = (TK - 1)t_\alpha$$

$$\text{or } \bar{t}_\alpha = t_\alpha - (T - \bar{t}_\alpha)K t_\alpha, \quad (3.7)$$

$$\bar{t}_\alpha = t_\alpha - \sum_{\beta \neq \alpha} \bar{t}_\beta K t_\alpha.$$

Equations (3.6) and (3.7) provide the desired expansion of T in t_α . The labels α may be ordered to form two sets such that for $\alpha > \frac{1}{2}N$, refers to electrons and for $\alpha \leq \frac{1}{2}N$ refers to ions. Therefore, t_α is an ion-atom or electron-atom t matrix, depending on α . However, \bar{t}_α mixes the two kinds beyond the first term. This mixing comes about because general m -body collisions, $m = 3, 4, \dots, N$, are being expanded in terms of two-body collisions. Hence, e.g., a three-body collision involving an ion, electron, and atom will require an ion-atom and an electron-atom t matrix.

The above allows expansion of the left side of (2.9) in two-body operators. In order to do so for the right-hand side, we must express $L_{1a}(\vec{E}_i) = \sum_\alpha L \times (\vec{E}_\alpha)$, in terms of the corresponding t' matrix:

$$t'_\alpha = iL(E_\alpha) + iL(E_\alpha)K_\alpha t'_\alpha. \quad (3.8)$$

This t' matrix differs from (3.5) for $\alpha \leq \frac{1}{2}N$ in the replacement of the exact two-particle L_α by the dipole approximation $L(\vec{E}_\alpha)$, $[L_{1a}(\vec{E}) = \sum_\alpha L \times (\vec{E}_\alpha)]$, and the replacement of K by K_α .¹⁴ Equation (3.8) may be solved for $L(\vec{E}_\alpha)$ to give

$$iL_{1a}(E) = - \sum_{\alpha=1}^{N/2} \sum_{p=0}^{\infty} t'_\alpha (K_\alpha t'_\alpha)^p. \quad (3.9)$$

Equations (3.4), (3.6), (3.7), and (3.9) allow the defining equation for $\mathcal{H}(w)$, (2.9), to be written in the desired form

$$K_a + K_a \langle T \rangle K_a$$

$$= \langle [w - iL_a + \sum_{\alpha=1}^{N/2} \sum_{p=0}^{\infty} t'_\alpha (K_\alpha t'_\alpha)^p - i\mathcal{H}(w)]^{-1} \rangle. \quad (3.10)$$

Suppose now that a parameter a is formally introduced by $t_\alpha \rightarrow at_\alpha$, $t'_\alpha \rightarrow at'_\alpha$. This corresponds in the simple case mentioned above to considering the t matrix to be proportional to a scattering length. This formal procedure is still meaningful here in the following sense. For long-range forces, the expansion (3.7) almost certainly does not converge. However, this expansion occurs

in (3.10) averaged over an equilibrium ensemble. This allows the potentials to become "dressed," or shielded, so that in effect they are finite ranged. Further, the scattering of interest to line broadening is predominantly that for which the atom is not ionized, so that although there is internal structure, the atomic electron remains in a small bounded region about the nucleus. Expanding left- and right-hand sides of (3.10) to first order in a gives $\mathcal{H}(w)$ to this order;

$$\mathcal{H}(w) = i \sum_{\alpha=1}^N \langle t_\alpha(w) \rangle - i \sum_{\alpha=1}^{N/2} \langle t'_\alpha(w) \rangle. \quad (3.11)$$

Since particles of the same species are indistinguishable (3.11) may be written

$$\mathcal{H}(w) = \frac{1}{2}iN \{ \langle t_e(w) \rangle + \langle [t_i(w) - t'_i(w)] \rangle \}. \quad (3.12)$$

Here, $t_e(w)$ and $t_i(w)$ represent, respectively, the single-electron-atom t matrix and the single-ion-atom t matrix. For particles without internal degrees of freedom and short-ranged forces $t_\alpha \sim 1/\Omega$, Ω =volume. Since the t matrices in (3.12) are averaged, it may be expected that they represent effective short-ranged forces, as discussed above. Therefore, (3.12) results from an expansion analogous to a density expansion [strictly speaking, (3.12) is not the leading term in a density expansion, since the statistical factor ρ_p , and therefore $\langle t_\alpha \rangle$, is density dependent]. Finally, the impact limit¹⁵ is given by

$$\mathcal{H}(0) = \frac{1}{2}iN \{ \langle t_e(0) \rangle + \langle [t_i(0) - t'_i(0)] \rangle \}, \quad (3.13)$$

which is the usual result with corrections to the dipole approximation.

The more general expression (3.12) is the desired result. This result is closely related to the "unified line-shape approximation" of Smith, Cooper, and Vidal. To make this relationship clear we may write, from (2.10),

$$J(w, \vec{g}) = -(\pi)^{-1} \text{Im} \text{Tr} \rho_a \vec{d} \cdot \langle C(w) \vec{d} \rangle,$$

$$[w - iL_a - iL_{1a}(\vec{g}) - i\mathcal{H}(w)]C(w) = 1,$$

or, in terms of the inverse transform of $C(w)$,

$$\frac{\partial}{\partial t} C(t) + L_0 C(t)$$

$$= - \int_0^t dt' \mathcal{H}(t-t') C(t'), \quad C(0) = 1,$$

$$L_0 = L_a + L_{1a}(\vec{g}).$$

Introducing an "interaction representation" by $C(t) = e^{-L_0 t} F(t) e^{L_0 t}$, we get

$$\frac{\partial}{\partial t} F(t) = - \int_0^t dt' \mathcal{H}_I(t, t') F(t'), \quad (3.14)$$

$$\mathcal{H}_I(t, t') = e^{L_0 t} \mathcal{H}(t-t') e^{-L_0 t'}.$$

This equation is formally the same as Eq. (25) of Ref. 10. It is exact, although not very practical. If the second term in (3.12), due to ion motion, is neglected Eq. (3.14) becomes

$$\begin{aligned} \frac{\partial}{\partial t} F(t) &= -\frac{1}{2}N \int_0^t dt' \langle L_{ea}(t) U(t, t') L_{ea}(t') \rangle F(t') \\ L_{ea}(t) &= e^{(L_0 + L_p)t} L_{ea}^1 e^{-(L_0 + L_p)t}, \\ U(t, t') &= T \exp \left[-\int_0^t dt'' L_{ea}(t'') \right]. \end{aligned} \quad (3.15)$$

Here, L_{ea}^1 is the interaction operator for one electron with the atom. This result is very close to the unified-line shape approximation, and indeed is the same as Eq. (50) of Ref. 10 under their assumptions of classical path and statistically independent quasiparticles. Thus, aside from the ion-motion terms in (3.12), our binary-collision result agrees with that of Ref. 10. The latter demonstrates that this result encompasses both the usual impact theory and the one-electron wing theory. It is felt that the binary-collision expansion technique clarifies some of the assumption involved in the impact approximation,¹⁵ first of all by providing a formal expansion to generate corrections. In addition, the assumption that collisions do not overlap in time is seen here to be related to the requirement of effective short-ranged forces, which is possible because t_α always occurs in an average over the plasma.

Finally, connection with the work of Kogan is possible. If one considers noninteracting perturbations, and classical dynamics, the result (3.12) is essentially exact. This may be seen by observing from (3.7) that corrections to the density expansion leading to (3.12) involve terms like

$$[\langle t_\beta K t_\alpha \rangle - \langle t_\beta \rangle K_\alpha \langle t_\alpha \rangle]_{\alpha \neq \beta},$$

which vanishes under the above assumptions. Thus, (3.12) is an exact result for the model considered by Kogan, although in quite a different form.

IV. RANDOM-PHASE APPROXIMATION

Sections II and III have been concerned with the description of the line shape for values of the frequency separation from the line center for which the dominant influence of the ions is a static-field effect. This was done by summing the important static-ion contributions explicitly in the microfield function, and the ion motion (as well as electrons) was treated in a perturbation approximation.

As the line center is approached these results can no longer hold since the static-ion contribu-

tion is dominated by the ion-motion effects. For these frequencies one must expect the perturbation expansions of Secs. II and III to break down as indicated by a sharp increase in the $\mathcal{H}(w)$ operator due to ion motion. The usual static-ion theories are unable to demonstrate this breakdown of the region of utility of the microfield function since the mechanism for ion motion is neglected from the outset. In this section the operator $\mathcal{H}(w)$ will be investigated further to show how this breakdown of the static-ion approximation is signaled. The form for $\mathcal{H}(w)$ obtained in Sec. II is given as a linear function of $G_{\mu\nu, \mu'\nu'}^R(w)$ defined by Eqs. (2.13) and (2.14). The plasma dynamics are contained in the dielectric constant $\epsilon(\vec{k}, w)$ whose form is not yet calculable in general. Here, we shall evaluate $G_{\mu\nu, \mu'\nu'}^R(w)$ in the random-phase approximation, for which the dielectric constant is known. In addition, a strong collision cutoff will be introduced for both ions and electrons, to make reasonable the use of the Born approximation of Sec. II. While this model has been justified to some extent for electron broadening, no corresponding study has been made to indicate its relevance when ions are included as well. We therefore emphasize that the results obtained here are not intended to be interpreted as quantitatively realistic but rather as a model which should be qualitatively accurate, and instructive as to the nature of the ion contribution.

The dielectric constant in the random-phase approximation for a two-component, nondegenerate plasma with uniform temperature is¹⁶

$$\begin{aligned} \epsilon(k, w) &= 1 + \left(\frac{1}{4} \beta w_{pe}\right)^2 (1/2x^3) [\phi(x + a/x) \\ &\quad + \phi(x - a/x) + \phi(x/\mu + a\mu/x) + \phi(x/\mu - a\mu/x) \\ &\quad + i\pi^{1/2} e^{-2a} (e^{4a} - 1) [I(x) + I(w/\mu)]], \end{aligned}$$

$$\phi(x) = e^{-x^2} \int_0^x dt e^{t^2}, \quad I(x) = e^{-x^2} \int_0^x dt e^{-t^2}, \quad (4.1)$$

where $a = \frac{1}{4} \beta w$ and $x = (\beta/8m)^{1/2} k$ are dimensionless variables, m is the electron mass, w_{pe} the electron plasma frequency, and μ is the ratio of the ion mass to the electron mass. It is sufficient for the purposes here to consider only the first term in (2.13), which will be denoted by $G_{\mu\nu, \mu'\nu'}(w)$.

$$\begin{aligned} G_{\mu\nu, \mu'\nu'}(w) &= (4\pi)^{-1} n(w) \\ &\quad \times \int \frac{dk}{k} \frac{\text{Im} \epsilon(k, w)}{|\epsilon(\vec{k}, w)|^2} A_{\mu\nu, \mu'\nu'}(k). \end{aligned} \quad (4.2)$$

Use of (4.1) in (4.2) gives two terms;

$$\begin{aligned} G_{\mu\nu, \mu'\nu'}(w) &= \frac{(\pi)^{1/2} \beta^2 n e^2}{32m} e^{-2a} \\ &\quad \times \left[\int_0^{x_0} \frac{dx}{x^4} \frac{I(x)}{|\epsilon'(x, w)|^2} A_{\mu\nu, \mu'\nu'}(x) \right. \end{aligned}$$

$$+ \int_0^{x_0} \frac{dx}{x^2} \frac{I(x/\mu)}{|\epsilon'(x, w)|^2} A'_{\mu\nu, \mu'\nu'}(x) \Big]. \quad (4.3)$$

The first term in (4.3) is due to electron motion and the second originates from ion motion. The upper limit on the integral results from the previously mentioned strong-collision cutoff and reflects the fact that both the random-phase approximation and (2.12) are inadequate for the strong collisions represented by large k (or x). This has been justified to a considerable extent, for the electron-broadening calculations, by Shen and Cooper⁸ who evaluate the average t matrix as an average over the impact parameters ($\sim 1/k$) in a classical-path approximation. They show that the t matrix oscillates sufficiently for small impact parameters to allow their contribution to be neglected, i. e., a small impact-parameter cutoff. They emphasize that this property is a result of their approximations preserving the unitarity of the t matrix. Unitarity is automatic in the binary-collision expansion given here, and it will be assumed that this qualitative behavior is still meaningful in some sense when the ion-motion terms are included as in (3.12).

The impact-parameter cutoff used here is that suggested in Ref. 8. For the corresponding range of x integrated over, $A'_{\mu\nu, \mu'\nu'}$ is well approximated by the first nonvanishing term of power-series expansion in x . The resulting contribution is that which would have been obtained if the dipole approximation were made from the outset. Closer analysis of the justification of the cutoff procedure, however, will require the formalism without the dipole approximation and is the reason for retaining all generality to this point. The resulting expression for $G_{\mu\nu, \mu'\nu'}^R(w)$ is proportional to a function $G(w)$,

$$G(w) = G_e(w) + G_i(w), \quad (4.4)$$

$$G_e(w) = \int_0^{x_0} \frac{dx}{x} \frac{I(x)}{|\epsilon(x, w)|^2},$$

$$G_i(w) = \int_0^{x_0} \frac{dx}{x} \frac{I(x/\mu)}{|\epsilon(x/\mu, w)|^2},$$

where the cutoff is $x_0 \cong 0.1$ (for a system with electron density and ion density of 3×10^{17} and temperature $T = 10^4$). These integrals have been evaluated numerically. The electron term differs from previous calculations¹⁷ only in a dip for small w . This occurs as a result of additional shielding (by the ions) included in the dielectric constant, and becomes effective approximately at values of w corresponding to the ion plasma frequency. The ion term is qualitatively the same only scaled differently by the mass change; thus the curve flat-

tens at the ion plasma frequency rather than the electron plasma frequency, and is multiplied by μ . The ion term goes to zero μ times faster than the electron term but is μ times greater. The sum of these two terms is given in Fig. 1. For $w \gtrsim 0.8 w_{pe}$, the static-ion approximation is valid. For smaller w the function rises sharply due to the ion-motion contributions. Even though the function eventually flattens out again at the ion plasma frequency this sharp increase marks the failure of the static-ion limit, and corresponding use of (2.10).

The onset of ion motion indicated above occurs for values of w about an order of magnitude larger than expected. This is probably due to the cutoff procedure not accurately accounting for strong ion-atom collisions. The utility of the simpler expansion of Sec. II thus requires a more detailed study of the ion cutoff, or better, evaluation of the strong-collision expression (3.12). $G(w)$ has been evaluated under the assumption that the ions and the electrons are in quasiequilibrium at different temperatures. If the ion temperature is taken to be one-tenth the electron temperature, the region of ion motion is reduced by roughly 50%.

V. DISCUSSION

The results of Sec. IV, although tentative, indicate the roles of the various descriptions of line shapes presented here. In the line center, both ions and electrons move appreciably and one expects (2.5) and (2.6) with $M(w)$ calculated by per-

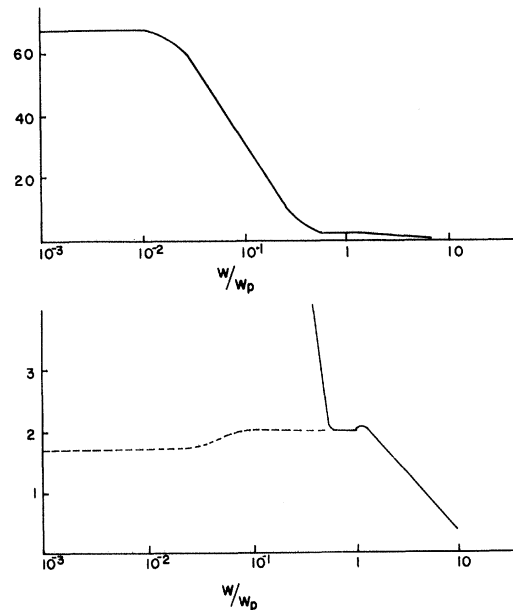


FIG. 1. Above: plot of $G(w)$ versus w/w_p for $T = 10^4$, $n = 3 \times 10^{17}$; below: same $G(w)$ showing detail of the onset of ion motion. Dashed curve is the contribution from $G_e(w)$ [see Eq. (4.4)].

turbation theory will provide an adequate description. Figure 1 shows that ion motion becomes less important at larger frequencies (beyond the ion plasma frequency). For larger frequencies the static-ion contributions dominate and should be summed by the introduction of the microfield distribution function. In this region, then, the results of Sec. II should be used. However, the treatment of perturber motion in a Born approximation is not adequate for close atom-perturber collisions. The proper treatment of these collisions was given in Sec. III. It is felt that this provides the necessary formalism to extend smooth-

ly the static-ion approximation to the line center. Meaningful line shapes in the region of interest here will be obtained following the determination of a more justified cutoff procedure for the ions, or evaluation of Eq. (3.12), presently under consideration.

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