Therefore, for a pair of distinguishable atoms the two contributions cancel, as the pair wave function contains equal parts of symmetrized and antisymmetrized components.]

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Electron Broadening of Isolated Spectral Lines*

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The electron broadening of an isolated atomic transition is calculated using the propagator approach. Electron correlations are included, and therefore the divergences arising in the impact-limit calculations are eliminated. The general expression for width reduces to previously obtained results if the correlations are neglected. The case of plasmon broadening is also considered. In this case, the width parameter has resonance-type frequency dependence, resulting in considerable deviation from Lorentz profile. Under suitable conditions "sidebands" appear about a "forbidden line."

I. INTRODUCTION

Broadening of atomic spectral lines in a plasma is of considerable interest at present. While a quasistatic approximation can be used for ion broadening, the dynamics must be considered for electron broadening.[1] The long-range Coulomb interaction causes special problems in the calculation of electron broadening in the impact limit, since a binary collision approximation is not strictly valid. Griem *et al.* employed a cutoff to avoid the divergence that arises in the linewidth calculation based on the impact limit.[2] Lewis further investigated the validity of these results and obtained a different cutoff, suitable for the wings of the line.[3] Recently, Smith and Hooper[4,5] treated the problem more generally, using the resolvent technique, and showed that the divergences do not arise. Moreover, the width parameter has an appreciable dependence on frequency, which leads to a deviation from a Lorentz profile, including asymmetry.

The purpose of this paper is to apply the "propagator technique" to the case of an isolated line. The necessary formalism has been developed in an earlier paper,[6] in which an application to resonance broadening was considered. (This paper will be referred to as I.) We derive a formula for the width parameter which includes the electron correlations; it does not involve any divergence. In the limit of no electron correlations, this formula reduces to the result of Griem *et al.*[2] near the line center, and to the result of Smith and Hooper[4] in the line wings.

We also consider the interesting case of the "plasmon broadening." In this case, the electron correlations give rise to collective excitations. The resulting width parameter has a resonance type of frequency dependence and the line shape is basically different. Under suitable conditions this line shape will exhibit fine structure. In particular, it could include "sidebands" about a neighboring "forbidden line." The possibility of such sidebands was earlier predicted by Baranger and Mozer[7] by calculating the probability of a second-order transition caused jointly by plasmons and photons. In our treatment this result arises as one of the consequences of "plasmon broadening."

The main advantage of the formalism employed in this paper is the automatic inclusion of all electron correlations. This makes the actual calculations simpler. In addition, contact is made with the standard work on the many-electron problem,[8,9] which permits the use of existing results to treat other interesting cases in electron broadening, e.g., the impurity spectrum in metals. Ion broadening can also be treated within this general framework, if the quasistatic approximation is not sufficient and ion dynamics should be included.

II. BASIC RELATIONS

In I, the general line-shape function was related to the irreducible "hole-particle propagator," χ. [See Eq. (6) and Fig. 1 in I.] Some of the diagrams which can contribute (in electron broadening) to the self-energy part Σ and the vertex function K are shown in Fig. 1. We shall consider only the first-order diagrams in the "effective interaction" since the contribution of higher-order diagrams is small. (We have also neglected the transverse photon propagator since its contribution is of the order of natural width.) The first-order diagram for K, shown in Fig. 1, results in a nonresonant contribution to the propagator χ

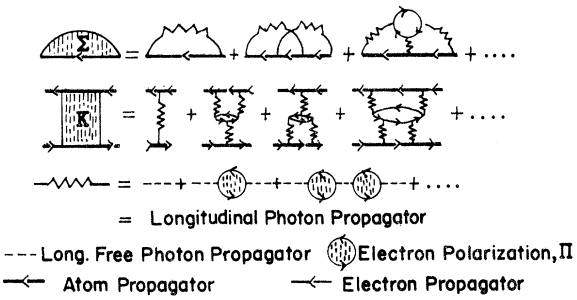

FIG. 1. Some of the diagrams for the self-energy and the vertex function, which are relevant to electron broadening, are shown. The longitudinal photon propagator includes all electron correlations. For example, if it is combined with the electronic charge and the atomic dipole moment, the result represents the "effective monopole-dipole interaction" between an electron and an atom.

and therefore K can be neglected for an isolated transition $\nu \to \mu$. (Its contribution is, however, important in the case of overlapping lines.) In this paper we shall calculate Σ_μ, which represents the width and shift parameter of the upper level μ. (Σ_ν can be calculated similarly, if desired.) The line shape is given by Eq. I-(12a), where I refers to the Ref. 6. Neglecting Doppler broadening and the velocity dependence of Σ_μ (which is negligible in electron broadening), this line-shape function is

$$\chi_{\mu\nu}{}^{0}(\Delta\omega_{\mu\nu}, \beta) = -2N_\nu \mathrm{Im}\left[\Delta\omega_{\mu\nu} - \Sigma_\mu(\omega, \beta)\right]^{-1}, \tag{1}$$

$$\Delta\omega_{\mu\nu} = \omega - \omega_{\mu\nu}, \quad \beta = 1/k_B T \ , \tag{2}$$

where N_ν is the number density of atoms in state ν.

The contribution to Σ_μ of the first diagram of Fig. 1 is the same as that considered in I. (See Fig. 2 of I.) Ignoring transverse interaction, taking the quantization axis along $\vec{q}$, and performing the angular integrations, we obtain from Eqs. I-(18a) and I-(16b)

$$\Sigma_\mu(\omega, \beta) \cong (i2/3\pi)\sum_{\mu'} |d_{\mu\mu'}|^2 [\exp(-\beta\Delta\omega_{\mu'\nu}) - 1]^{-1} \int_0^\infty dq\, q^2 \ \mathrm{Im}\left[\epsilon(q, -\Delta\omega_{\mu'\nu} + i\delta)\right]^{-1}. \tag{3}$$

In (3) ϵ is the longitudinal dielectric constant of the electron gas; $d_{\mu\mu'}$ is the dipole matrix element for the transition $\mu \to \mu'$, caused by the perturbing electron, and $\delta \to 0_+$. (The small kinetic factors in Eq. I-(18b) are ignored since the electron momentum $\ll$ the momentum of the atom; these kinetic factors are responsible for the velocity dependence of Σ_μ in resonance broadening.) The dominant perturbation of the atom results from the monopole-dipole interaction with an electron.

Equation (3) includes the second-order monopole-dipole interaction together with the electron-electron correlations contained in ϵ. We shall use the random phase approximation (RPA) for ϵ,[8,9] since it includes the correlations important for our problem. In this approximation, the polarization (Π in Fig. 1) results from the free "electron-hole propagator," and we have

$$\epsilon(q, \Delta + i\delta) = 1 + (4\pi e^2/q^2) \int [d\vec{p}\,/(2\pi)^3] \left[n(\vec{p} + \vec{q}/2) - n(\vec{p} - \vec{q}/2)\right] / (\Delta - \vec{p}\cdot\vec{q}/m + i\gamma) \ , \tag{4}$$

$$n(\vec{p}) = \{\exp\left[\beta(p^2/2m - U)\right] + 1\}^{-1} \ , \tag{5}$$

where e and m denote the charge and mass of an electron, and U is the chemical potential; γ represents the damping of the pair propagator state, and in RPA $\gamma \to 0$. Now we specialize to two different physical situations.

III. ELECTRON BROADENING

Here we consider the case in which the effect of collective plasmon excitations is not important. Let $\omega_p = (4\pi ne^2/m)^{1/2}$ denote the plasma frequency, where n denotes the total electron number density. When $\Delta \ll 1/\beta$, the following approximation is obtained from (4).

$$\epsilon(q, \Delta + i\delta) \cong 1 + (q_D/q)^2 + i(q_D{}^2\, \bar{p}/2q^3)\exp\left[-\beta(\Delta m/q + q/2)^2/2m\right](e^{\beta\Delta} - 1) \ , \tag{6a}$$

$$q_D = (4\pi ne^2\beta)^{1/2} = 1/L_D, \quad \bar{p} = (2\pi m/\beta)^{1/2} \ , \tag{6b}$$

where L_D is the Debye length. In obtaining (6a), we have replaced the Fermi function in (5) by the Boltzmann distribution function. Substituting $y = \beta q^2/8m$, we obtain from (3) and (6a):

$$\Sigma_\mu(\omega,\beta) = -i(2ne^2/3)(8\pi m\beta)^{1/2}\sum_{\mu'}|d_{\mu\mu'}|^2\exp(\beta\omega_{\mu'\nu}/2)I(\Delta\omega_{\mu'\nu}), \tag{7}$$

$$I(\Delta\omega_{\mu'\nu},\beta) = \tfrac{1}{2}\int_0^\infty (dy/y)\exp\left(-y-\beta^2\Delta\omega_{\mu'\nu}^2/16y\right)\Big[(1+\pi\alpha^2/4y)^2 + (\pi^3\alpha^4/64y^3)\exp\left(-2y-\frac{\beta^2\Delta\omega_{\mu'\nu}^2}{8y}\right)\sinh^2\left(\frac{\Delta\omega_{\mu'\nu}}{2}\right)\Big]^{-1}, \tag{8a}$$

$$\alpha = q_D/\bar{p} = \bar{\lambda}/(2\pi L_D) = (2\pi)^{-1/2}\beta\omega_p, \tag{8b}$$

where $\bar{\lambda}$ is the thermal de Broglie wavelength $= h/\bar{p}$. (We have been using units with $\hbar = 1$.) Equation (7) gives the width parameter and should be valid both in the line core as well as the wings provided that $\Delta\omega_{\mu'\nu} \ll 1/\beta$.

The parameter α is a measure of the contribution of electron correlations. When $\alpha \to 0$, the correlations are negligible, and we obtain

$$I(\Delta\omega_{\mu'\nu},\beta) = \tfrac{1}{2}\int_0^\infty dy\, y^{-1}\exp(-y-\beta^2\Delta\omega_{\mu'\nu}^2/16y) \quad = K_0(\beta\Delta\omega_{\mu'\nu}/2), \tag{9}$$

where K_0 denotes the modified Bessel function. Equations (7) and (9) give the same result as that obtained by Smith and Hooper by a very different procedure. [See the first term in Eq. (57) of Ref. 4, noting that $K_0(z) = (-i\pi/2)H_0^{(2)}(-iz)$; the second and third terms represent the contribution of Σ_ν and the coupling K. For an isolated transition only the "diagonal part" of this result is required; therefore the third term vanishes. This justifies the neglect of the first-order diagram for K in Fig. 1.] When $\beta\Delta\omega_{\mu'\nu} \ll 1$, (9) reduces to a result similar to that obtained by Lewis.[3]

$$I(\Delta\omega_{\mu'\nu},\beta) \cong -0.577 - \ln(\beta\Delta\omega_{\mu'\nu}/4). \tag{10}$$

Equations (9) and (10) diverge as $\Delta\omega_{\mu'\nu} \to 0$. In this region the full expression (8a), in which the contribution of electron correlations eliminates the divergence, should be used. In fact if we set $\Delta\omega_{\mu'\nu} = 0$ in (8a), the result is

$$I(\beta) = \tfrac{1}{2}\int_0^\infty dy\, e^{-y}y^{-1}(1+\pi\alpha^2/4y)^{-2}. \tag{11}$$

If the effect of correlations is neglected now by setting $\alpha = 0$, we obtain

$$I = \tfrac{1}{2}\int_{y_{\min}}^\infty dy\, e^{-y}/y, \tag{12}$$

where the divergent integral has been cut off at $y_{\min}$. Equations (7) and (12) give precisely the same linewidth as that obtained by Griem *et al.*, in classical path and impact approximation. [See Eq. (29) of Ref. 2.] In Eq. (11), the contribution of the electron correlation eliminates the divergence and, consequently, the necessity of the cutoff at $y_{\min}$.

To summarize, if $\bar{\lambda} \ll L_D$, Eq. (9) or (10) should be valid in the wings, whereas (12) should be valid near the line center. In both, the effect of electron correlations is neglected. When this effect is important ($\bar{\lambda} \sim L_D$), the expressions (8a) or (11) should be used. Smith also obtained a correction to (9) which takes into account the electron correlations. Because his result has a very different form, an immediate comparison with (7) is not possible. [See Eqs. (5) and (7) of Ref. 5. Note that (7) involves an integration over "time variable" while in our Eq. (8a), $y = \beta q^2/8m$, where q represents momentum transfer.]

IV. PLASMON BROADENING

If $\Delta\omega_{\mu'\nu} > 1/\beta$, the plasmon excitation should be considered, in addition to the single-particle behavior of the perturbing electron gas. This is a limiting case of electron correlations. In this situation the appropriate approximation for ϵ, as obtained from (4), is

$$\epsilon(q,\Delta) = 1 - \omega_p^2/\Delta^2 + i(\pi me^2/q^3)(8\pi m\beta)^{\frac{1}{2}}\exp[-(\beta/2m)(\Delta m/q + q/2)^2](e^{\beta\Delta} - 1). \tag{13}$$

The Imϵ is the same as in (6a) and represents the "damping" of the plasmons. From (3) and (13) we obtain

$$\Sigma_\mu(\omega,\beta) = -i(\tfrac{2}{3}ne^2)(8\pi m\beta)^{\frac{1}{2}}\sum_{\mu'}|d_{\mu\mu'}|^2 \exp(\beta\omega_{\mu'\nu}/2)\, K_0(\beta\Delta\omega_{\mu'\nu}/2)/\{[1-(\omega_p/\Delta\omega_{\mu'\nu})^2]^2+\eta^2\}\,. \tag{14}$$

In evaluating the integral over q, we have set Im $\epsilon = \eta$, only in the denominator. Thus q dependence of the plasmon damping is ignored by using an average value η. Then result (9) was used to obtain (14). This procedure should be valid if $\Delta\omega_{\mu'\nu}$ is large and the damping is small. [When $\Delta = \omega_p$, a better approximation[8] for ϵ should be used, in place of (13).]

Equation (14) contains the resonance-type dependence of Σ_μ on ω. If several levels μ' are close to each other, the resulting line shape, given by Eq. (1), will deviate appreciably from a Lorentz profile, and may involve asymmetry. For a somewhat larger spacing of levels, μ', the line shape may exhibit "fine-structure." In particular, if there is one, well separated level, μ' with $\Delta\omega_{\mu'\nu} \cong \omega_p$, "sidebands" would appear at $\omega \cong \omega_{\mu'\nu} \pm \omega_p$, that is, on either side of the "forbidden transition," $\nu \to \mu'$. Baranger and Mozer[7] made a direct calculation of the probability of the second-order photon-plasmon transition $\nu \to \mu \to \mu'$. However, they did not obtain the line shape, because they were interested only in the "intensities" of the sidebands. With the help of (1) and (14), we obtain the profile from which the relative intensities of the main transition $\nu \to \mu$ and those of the sidebands follow directly. Furthermore, Eqs. (3) and (13) give the more general result for the case in which plasmon damping cannot be considered a constant. [However for an adequate treatment of the sideband "peaks" (at $\omega = \omega_{\mu'\nu} \pm \omega_p$) a better approximation[8] for ϵ must be used; moreover the damping of the intermediate state of the atom, represented by Im $\Sigma_{\mu'}$, should also be considered.[6]]

V. CONCLUSIONS

The electron broadening of an isolated atomic transition was calculated, using the propagator approach. The electron correlations were taken into account. The improvement over the impact-limit calculations removes the divergence that arises as a result of the long-range Coulomb interaction. The results obtained by Griem *et al.*,[2] and Smith and Hooper[4] were recovered in the limit of no electron correlations from the more general formula given by Eq. (7).

The case of plasmon broadening was also considered. In this case the line shape can have fine structure. In particular, the result of Baranger and Mozer[7] follows from the profile of the plasmon-broadened line.

The formalism, of course, is much more general. The key quantity is the longitudinal dielectric constant of the electron gas, which can be calculated in any desired approximation. Several useful approximations for it are well known in the literature on the many-electron problem.[8,9] For example, the case of a degenerate electron gas may be of interest in connection with the impurity spectra in metals. Moreover, the same formalism can also be applied to ion broadening, when the quasistatic approximation is not sufficient.

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