Evaluation of Electron-Atom Bremsstrahlung from Elastic Scattering*

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Asymptotic wave functions together with a perturbation-theoretic treatment of the long-range polarization effects are used to provide an analytic expression for the dipole-length matrix element for electron–neutral-atom bremsstrahlung. This result permits the evaluation of bremsstrahlung from elastic scattering phase shifts at the initial and final electron energy and from the static polarizability of the atom. The expression is approximate and contains a weak dependence on a cutoff parameter, but it provides a complete generalization of the formulas due to Low, and to Kas'yanov and Starostin, and it contains terms of all orders in the photon energy. The result is that, by substitution into the formulas, the bremsstrahlung cross section may be evaluated to within a few percent for nearly all the energy range tested, once the elastic scattering phase shifts have been determined.

Efforts to extrapolate information obtained from elastic scattering to processes off the energy shell have met with partial success, both in electron–neutral-atom and nucleon-nucleon bremsstrahlung. For both systems, it has been possible to obtain an approximation to the bremsstrahlung cross section in the soft photon limit from a knowledge of the elastic scattering phase shifts.[1–4] A previous calculation of electron-atom bremsstrahlung[5] presented an approximation giving the sp cross section as a function of the elastic scattering phase shifts at the initial and final electron energies, without restriction on the photon energy. It was shown that for oxygen and nitrogen the approximation is fairly successful in representing the total bremsstrahlung cross section for photon energies as high as 80% of the initial electron energy.

The present work generalizes the approximate expression of Ref. 5, hereafter referred to as I, to arbitrary electron angular momentum. Moreover, for other than sp transitions, the long-range effects of the polarization potential on the bremsstrahlung cross section are included by means of perturbation theory. The result is an expression giving the total bremsstrahlung cross section as a function of the elastic scattering phase shifts at the initial and final electron energies and of the static dipole polarizability of the atom.

In I, it is assumed that the system wave function may be adequately represented as the antisymmetrized product of a free wave and of the ground configuration of the atom; it is also assumed that the free orbitals are orthogonal to the ground state. This permits the calculation of the bremsstrahlung to be reduced to the evaluation of single free-particle radial dipole-length matrix elements of the form

$$(\tilde{\Lambda}_l^{l'})_{\mathcal{L}} = \tfrac{1}{2}(k_0^2 - k^2)^2 \times \int_0^\infty dr\, e^{-\epsilon r} r R_{l'}(kr) R_l(k_0 r)\,, \tag{1}$$

where the dependences on the total spin and angular momentum quantum numbers L and S, have been suppressed. For sp transitions, this quantity has been adequately evaluated from asymptotic wave functions, and the result is given in Eq. (21) of I. For that case, a finite soft-photon limit exists, since the apparent quadratic zero of Eq. (1) at zero photon energy is canceled by a quadratic resonance of the integrand. However, when both l and l' are ≥ 1, the method of I cannot be used to evaluate the matrix element, because the asymptotic wave functions contain the irregular Bessel functions n_l, which cause the integral to diverge at the origin. In addition, the polarization potential forces the wave function to reach asymptotic form very slowly, with the result that an appreciable nonasymptotic contribution to the matrix element comes from regions at some distance from the atom.

On the other hand, since the dipole-length matrix element is relatively insensitive to the wave function at small r, the effect of the core poten-

tials, both direct and exchange, is primarily to influence the building up of the phase shift. Similarly, if the polarization is taken into account through a close-coupling approach, its effect is mainly to distort the wave function at small r, and hence, it only indirectly influences the dipole-length matrix element through the phase shifts. In calculations that explicitly contain an r^{-4} potential, and also in an exact treatment of the scattering, the polarization effect is long range and must be included specifically, as is done here.

The method proposed here for evaluating this matrix element exploits the fact that the values of the wave functions for small r need not be calculated correctly. Thus, the wave function is taken to be the sum of its asymptotic form y_l and a perturbation z_l, which is assumed to be contributed by the polarization potential. Specifically,

$$r^{-1}R_l(kr) = y_l(kr) + z_l(kr) , \tag{2}$$

where the asymptotic wave function has the standard form

$$y_l(kr) = \cos\delta_l(k) j_l(kr) - \sin\delta_l(k) n_l(kr) , \tag{3}$$

and z_l is obtained by substituting Eq. (2) in the differential equation for $R_l(kr)$. To lowest order, this yields the defining equation

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right) z_l(kr) = -\frac{\alpha}{r^4}\, y_l(kr), \tag{4}$$

with the boundary condition

$$\lim_{r\to\infty} z_l(kr) = 0. \tag{5}$$

In keeping with the perturbation-theoretic definition of the quantities z_l and $z_{l'}$, the matrix element is evaluated to first order only in these quantities. The lower limit of the integral in Eq. (1) is then cut off at $r = b$; i.e., it runs from b to ∞. The cutoff should be large enough so that the assumed form of the wave function is reasonable, and small enough so that the major contributions to the integral have been included. In addition, the integral should be insensitive to the precise value adopted for b. These objectives appear to be met by the choice

$$k_0^2 = \alpha/b^4 , \tag{6}$$

where α is the static polarizability of the atom, k_0 is the initial electron wave number, and, in the following, k corresponds to the final electron energy. This definition of b marks a rough boundary for the validity of Eq. (4) for z_l. Clearly, a small change in Eq. (6) should alter b only slightly. Finally, the dependence of the matrix element on the nonphysical parameter b is minimized by setting $b = 0$ in all the terms which do not diverge in that limit. Thus, for $l, l' \geq 1$ the matrix element is evaluated from the equation

$$\begin{aligned}(\tilde{\Lambda}_l^{l'})_{\mathcal{L}} = \tfrac{1}{2}(k_0^2 - k^2)^2 \{ & \int_0^\infty dr\, r^3 [\cos\delta_l(k_0)\cos\delta_{l'}(k) \\ & \times j_l(k_0 r) j_{l'}(kr) - \cos\delta_l(k_0)\sin\delta_{l'}(k) j_l(k_0 r) n_{l'}(kr) \\ & - \sin\delta_l(k_0)\cos\delta_{l'}(k) n_l(k_0 r) j_{l'}(kr)] \\ & + \int_b^\infty dr\, r^3 [\sin\delta_l(k_0)\sin\delta_{l'}(k) n_l(k_0 r) n_{l'}(kr) \\ & + y_l(k_0 r) z_{l'}(kr) + z_l(k_0 r) y_{l'}(kr)]\} , \end{aligned} \tag{7}$$

where b is given by Eq. (6).

This then is, in outline, the extension of the formulation obtained in I. This equation can also be used for sp transitions if the second integral is set equal to zero, and this, in fact, reproduces the results of I. The reasons for excluding the second integral if l or $l' = 0$ are twofold: First, the $n_l n_{l'}$ term converges to zero when $b = 0$, and hence by the above rule should be neglected; second, the structure of the terms proportional to z_l and $z_{l'}$ depends upon the assumption that the integrand is well approximated by wave functions consisting, as indicated in Eq. (2), of an asymptotic part and a part determined by the polarization potential. This is manifestly incorrect for s waves, which have large amplitude in the core region. Only the existence of an angular momentum barrier makes such a decomposition reasonable. The nonasymptotic contributions to sp transitions thus seem difficult to evaluate; since their influence on the cross section is small, it seems best to drop them entirely.

An explicit representation of z_l is necessary in order to evaluate Eq. (7). A solution of Eq. (4), subject to the boundary condition of Eq. (5), is provided by the Green's function

$$G_l(k, r, r') = k[j_l(kr_<) n_l(kr_>) - n_l(kr) j_l(kr')], \tag{8}$$

with the result that

$$z_l(k_0 r) = -\alpha \int_r^\infty \frac{ds}{s^2}\, G_l(k_0, r, s)\, y_l(k_0 s) . \tag{9}$$

When the b-independent integrals are done explicitly and the b-dependent integrals are reduced to quadratures, the dipole-length matrix element takes the form

$$(\tilde{\Lambda}_{ll'})_{\mathcal{L}} = A_{ll'}\cos\delta_l(k_0)\cos\delta_{l'}(k) + B_{ll'}\cos\delta_l(k_0)\sin\delta_{l'}(k) + C_{ll'}\sin\delta_l(k_0)\cos\delta_{l'}(k) + D_{ll'}\sin\delta_l(k_0)\sin\delta_{l'}(k) \quad , \tag{10}$$

where, when $l' = l+1$,

$$A_{ll'} = -\tfrac{1}{2}\alpha(k_0^2 - k^2)^2 \int_b^\infty dr\, r^3 \int_r^\infty \frac{ds}{s^2} \times [G_l(k_0, r, s) j_{l+1}(kr) j_l(k_0 s) + G_{l+1}(k, r, s) j_l(k_0 r) j_{l+1}(ks)];$$

$$B_{ll'} = \tfrac{1}{2}\left(\frac{k_0}{k}\right)^l \left[\left(\frac{k_0^2 - 3k^2}{k^2}\right) + 2l\left(\frac{k_0^2 - k^2}{k^2}\right)\right] - \tfrac{1}{2}\alpha(k_0^2 - k^2)^2 \int_b^\infty dr\, r^3 \int_r^\infty \frac{ds}{s^2} \times [G_l(k_0, r, s) n_{l+1}(kr) j_l(k_0 s) + G_{l+1}(k, r, s) \times j_l(k_0 r) n_{l+1}(ks)];$$

$$C_{ll'} = \left(\frac{k}{k_0}\right)^{l+1} - \tfrac{1}{2}\alpha(k_0^2 - k^2)^2 \int_b^\infty dr\, r^3 \int_r^\infty \frac{ds}{s^2} \times [G_l(k_0, r, s) j_{l+1}(kr) n_l(k_0 s) + G_{l+1}(k, r, s) n_l \times (k_0 r) j_{l+1}(ks)]; \tag{11}$$

and

$$D_{ll'} = \tfrac{1}{2}(k_0^2 - k^2)^2 \left(\int_b^\infty dr\, r^3 n_l(k_0 r) n_{l+1}(kr) - \alpha \int_b^\infty dr\, r^3 \int_r^\infty \frac{ds}{s^2} G_l(k_0, r, s) n_{l+1}(kr) n_l(k_0 s) + G_{l+1}(k, r, s) n_l(k_0 r) n_{l+1}(ks)] \right) .$$

When $l = l' + 1$, the coefficients are evaluated from Eq. (11) by interchanging k and k_0 and replacing l by l'. If either l or $l' = 0$, the integral terms are dropped from Eq. (11).

It should be noted that in the above expressions the double integrals multiplying α are all convergent and are readily evaluated numerically. However, the single integral forming the first term of $D_{ll'}$ is semiconvergent and is evaluated, as usual, by introducing the wave-packet normalization factor $e^{-\epsilon r}$ and evaluating the integral as $\epsilon \to 0$. The result is that this integral may be expressed as a finite sum of products of Bessel functions evaluated at $r = b$. In all cases, the various integrals may be evaluated as definite functions of the electron energies and angular momenta, without reference to any particular electron-atom collision.

The bremsstrahlung cross section is then obtained, as in Eqs. (15) and (16) of I, namely, by

$$\sigma = \textstyle\sum_0 \pi a_0^2 / h\nu \ , \tag{12}$$

where $\sum_0 = \left(\frac{8}{3\pi}\right)\left(\frac{e^2}{\hbar c}\right)^3 \frac{k}{k_0} \sum_l \sum_S \sum_{LL'} \frac{2S+1}{2(2s_2+1)}$

$$\times [(2L+1)(2L'+1)/(2l_2+1)] W^2(l'L'lL\,|\,l_2 1) \times (l+1)[|\tilde{\Lambda}_{LSl}^{L'Sl+1}|^2 + |\tilde{\Lambda}_{LSl+1}^{L'Sl}|^2] . \tag{13}$$

It is clear that in the soft-photon limit the polarization correction vanishes, and to lowest order the bremsstrahlung cross section may be evaluated from the momentum-transfer cross section σ_m by

$$\textstyle\sum_0 = 4/3\pi^2 (e^2/\hbar c)^3 k_0^2 \sigma_m \ . \tag{14}$$

The usual first-order term is, of course, also readily derived. Thus, Eqs. (10)–(13) form a complete generalization of the various approximate soft photon theorems found previously by so many authors.[1-7] There is no restriction whatsoever on the photon energy in these formulas. On the other hand, as noted earlier, the results are not exact, and because of the approximations made in evaluating the free orbitals, there will be nonzero corrections even of order $(k_0^2 - k^2)^2$ or $(h\nu)^2$.

It is of interest to compare the above method for evaluating electron-atom bremsstrahlung with the quantum defect method,[8-10] as applied to the evaluation of electron-ion bremsstrahlung.[11] Both methods agree in the number of phase shifts and matrix elements which should be introduced to describe the bremsstrahlung process, since the quantum defect method is also capable of allowing for the angular momentum of the target atom via L-S coupling.[9,11] However, the two methods differ in the asymptotic wave functions used to represent the free orbitals, in the procedures used to evaluate the relevant integrals, and in the values taken for the phase shifts.

The quantum defect method (QDM) represents the free orbitals as a linear combination of undistorted Coulomb wave functions, with the irregular Coulomb solution being multiplied by an exponential cutoff factor containing an angular momentum dependent cutoff parameter $\tau_l^{-1} \approx [l(l+1)]^{1/2}$. In contrast, the present method introduces polarization-distorted spherical Bessel functions for the free orbitals and uses a sharp cutoff for the irregular solution (the cutoff parameter b being energy-dependent). Including the polarization distortion is essential in the electron-atom case, since these distortions occur at large r and affect the dipole-length matrix elements. These distortions should be less important in electron-ion scattering be-

cause the polarizabilities are smaller in this case and because the effect may be dominated by the Coulomb potential. Apparently no one has verified directly whether polarization distortion can be significant in electron-ion scattering.

The difference between an exponential and a sharp cutoff procedure is one of detail only. However, the latter procedure is simpler, since a number of integrals may then be evaluated in finite form. The principal difference in the two methods in this respect is in the value chosen for the cutoff parameter, and this difference is essential. In all cases, the rather small differences between the correct and the asymptotic wave functions become greatly enhanced, and the evaluation of $(\tilde{\Lambda})_{\mathcal{L}}$ is seriously affected, at small r values, where the irregular solutions have their region of polynomial growth. For the electron-ion case, the strong action of the Coulomb potential suffices to confine this region of growth to regions of the order τ_l^{-1}, with the result that $(\tilde{\Lambda})_{\mathcal{L}}$ is comparatively insensitive to this effect. In electron-atom scattering wave-function growth occurs over the much larger region $r \lesssim k^{-1}[l(l+1)]^{1/2}$, and major distortions in the value of $(\tilde{\Lambda})_{\mathcal{L}}$ occur. The present procedure for choosing b goes far toward excluding regions of nonphysical growth of wave functions, but it is certainly likely that this procedure leads to inaccurate values for $(\tilde{\Lambda})_{\mathcal{L}}$ at very low electron energies. The results of this effect for electron-hydrogen scattering are discussed in detail below.

A further difference in the evaluation of $(\tilde{\Lambda})_{\mathcal{L}}$ between the QDM and the present theory lies in the additional approximation, made in the QDM but not here, of using regular solutions only to evaluate radial integrals that depend on both the regular and irregular solutions. Specifically, in the QDM, approximate relations are used to express $(\tilde{\Lambda})_{\mathcal{L}}$ in terms of an amplitude G and a phase χ that are related by

$$G\cos\pi\chi = (k_0^2 - k^2)\int_0^\infty dr\, r F_l(k_0 r) F_{l'}(kr)\ ,$$

which contains regular Coulomb functions only. The phase is then adjusted to vary smoothly, and the amplitude is obtained from this relation. The result is to smooth out some of the nonphysical effects coming from the use of asymptotic wave functions, and is analogous to what is done in the present work for pd transitions at high photon energies. However, no critical analysis of the approximations made in evaluating the QDM radial integrals seems to have been made.

Finally, the two methods differ in the values for the phase shifts used in asymptotic wave functions, although, as will be pointed out below, this is not essential. The present method leaves these values completely open, allowing the phase shifts to be determined by any procedure whatever (scattering theory, variational technique, etc.), permitting the accurate evaluation of the bremsstrahlung cross section to become an additional test of the quality of the phase shifts. In contrast, the QDM provides a completely rigid procedure for evaluating these phase shifts from spectral data. In practice, this procedure is usually simplified by taking each phase shift to be of the form $\delta = a + bk^2$, and determining a and b empirically. The advantage of this is that only spectral data, and not an accurate scattering theory, is required for the evaluation of bremsstrahlung. The disadvantage is that the phase shifts are not necessarily good ones (in fact, for electron-atom scattering the above representation is quite poor), while the bremsstrahlung cross section is quite sensitive to small differences in the relative sizes of phase shifts. It is emphasized, however, that although the QDM prescription for phase shifts is usually taken to be the essence of the method, the prescription could be abandoned and the QDM expressions could be used with completely arbitrary phase shifts, as in the present method: This procedure would have a number of advantages of flexibility and would be quite attractive, once it is established that the QDM approximations for the radial integrals are adequate.

Before assessing the accuracy of these results, it is useful to make some comments on the dipole-velocity matrix element $(\tilde{\Lambda})_{\mathcal{V}}$, since at present the comparison of this matrix element with $(\tilde{\Lambda})_{\mathcal{L}}$ provides the most sensitive test of the accuracy of the bremsstrahlung calculation. Of course, if exact wave functions were available, these two matrix elements would be equal. When wave functions satisfying an approximate scattering theory are used, the agreement between the two matrix elements will in general be a useful test of the scattering theory for wave functions of high accuracy. For Hartree-Fock-like theories, the relation between the two matrix elements is given in the notation of I by

$$\begin{aligned}(\tilde{\Lambda}_l^{l'})_{\mathcal{V}} = (\tilde{\Lambda}_l^{l'})_{\mathcal{L}} + \tfrac{1}{2}(k_0^2 - k^2)\Big[\int_0^\infty dr\, r R_{l'}(kr) \\ \times R_l(k_0 r)[V_{l'}(r) - V_l(r)] + \sum_{j=1}^{\hat{N}} [R_l(k_0 r)\lambda_j^{l} - R_{l'} \\ \times (kr)\lambda_j^{l'}] R_{n_j l_j}(r) + \int_0^\infty dr\, r^2 \int_0^\infty dr' r'^2 \\ \times R_l(k_0 r) R_{l'}(kr') \left(\frac{J_{l'}(r, r')}{r'} - \frac{J_l(r', r)}{r}\right)\Big].\end{aligned}$$

It is seen that in general the two matrix elements agree in the soft-photon limit only. For larger photon energies, good agreement will occur only when the wave functions are fairly accurate; then the individual large terms of Eq. (15) will tend to

cancel. Of course, in the case of a pure potential scattering theory these correction terms are identically zero.

It is the dipole-velocity matrix element that follows directly from perturbation theory, and thus gives most directly the full content of the scattering theory. When the two matrix elements are in close agreement, it is the dipole-velocity element that provides the best estimate of the bremsstrahlung cross section. For this reason, in the figures below, the dipole-velocity calculation is used as the standard against which other calculations are compared. However, $(\tilde{\Lambda})_v$ is very sensitive to the values of the wave function for small r, and may even have the wrong order of magnitude unless the wave functions are quite accurate. When the two matrix elements markedly disagree, it is probably best to accept $(\tilde{\Lambda})_\ell$ as providing the best estimate of the bremsstrahlung; and this is in fact usually done in the literature. The basic reason for this is that $(\tilde{\Lambda})_\ell$ is sensitive primarily to the elastic scattering phase shifts, and these phase shifts have usually been obtained from a scattering theory which has been chosen for its ability to represent experimental elastic scattering data. Thus, $(\tilde{\Lambda})_\ell$ is usually more directly constrained by experiment.

The results of applying the theory of I and the expressions of the present paper to the evaluation of bremsstrahlung emission from collisions of electrons and neutral hydrogen atoms is given in Fig. 1. The solid curves represent the dipole-velocity calculations and are thus the standard for comparison. The separate sets of curves are labeled with the initial electron energy. The short-dashed curves represent the exact evaluation of the dipole-length matrix elements, while the long dashes give the result obtained from the expressions of the present paper.

Since the analytic approximation is designed to represent the dipole-length result, the fact that it agrees more nearly with the dipole-velocity calculation must be the fortuitous result of cancellation between the $^1\Sigma_{sp}$ and the $^3\Sigma_{sp}$ curves, which

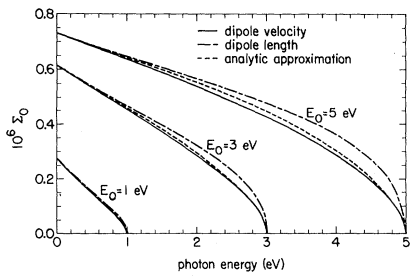

FIG. 1. Calculated values of Σ_0 for electrons on neutral hydrogen. The total bremsstrahlung cross section is obtained from Σ_0 by use of Eq. (12).

lie, respectively, above and below the dipole-velocity curve.

It is seen that for electron-hydrogen scattering the scattering theory of I provides an accurate evaluation of the bremsstrahlung, according to the usual criterion of agreement between the dipole-length and the dipole-velocity cross sections. In addition, the use of the phase shifts and polarizability from the theory of I in the formulas developed here, leads to good agreement with the results of the full numerical evaluation, with the differences being only a few percent over the entire energy range of interest. Although the present theory has been compared with I only, it is expected that there will be comparable agreement in general. Thus, the consequences of any scattering theory for the prediction of bremsstrahlung may be assessed once the elastic scattering phase shifts are known. For example, variational techniques[12–14] could be used to obtain the phase shifts despite the fact that these techniques usually yield rather poor wave functions near the core of the atom. There is in principle a difficulty in obtaining an α which is consistent with the phase shifts adopted, but with the present range of uncertainties in α values (about 10–15%), such difficulties would introduce only a 1–2% variation in the bremsstrahlung cross section in the cases studied.

Of course, Fig. 1 shows only that the present theory reproduces the full result of a scattering theory quite closely, and that the scattering theory of I meets the usual requirement for an accurate evaluation of the bremsstrahlung cross section. It does not guarantee that any of the curves displayed there provide bounds for the physical values of this cross section, or that they even have a close relation to them: Such guarantees are provided only by knowledge that the phase shifts inserted into the present theory are essentially exact, whereas good agreement between $(\tilde{\Lambda})_\ell$ and $(\tilde{\Lambda})_v$ is merely a necessary consequence of accurate wave functions and is not a highly sensitive test of the quality of the phase shifts. This point is presently being studied in more detail, using the present theory to evaluate the consequences of various scattering theories; the results will be reported later.

In Figs. 2–5, the results are displayed separately for the singlet and triplet sp and pd contributions to Σ_0. It is seen that in general the present theory gives a reasonably good value for the individual terms, with the exception of the $^1\Sigma_{pd}$. However, this last is so small that numerical uncertainties in the calculation begin to be important. Moreover, due to the small size of the singlet p-wave phase shift, the b-dependent correction is significant over a larger energy range, and hence the cutoff of the integrals in the perturbation calculation becomes more critical. The same problems plague $^3\Sigma_{pd}$ at the highest pho-

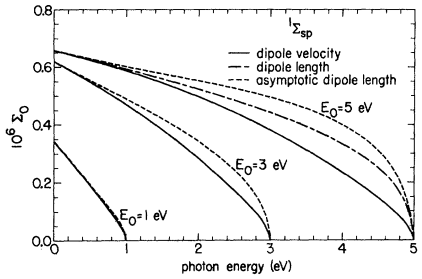

FIG. 2. Σ_0 for singlet *sp* transitions.

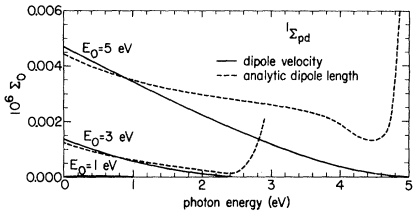

FIG. 4. Σ_0 for singlet *pd* transitions.

ton energy. The correct cross section vanishes through cancellation between the asymptotic part and the remainder, so once again the result is sensitive to the cutoff. In plotting Fig. 1, the *pd* contribution to $\sum_0$ was set to zero for photon energies equal to the initial electron energy.

The deviations in the $^3\Sigma_{sp}$ curves are primarily due to the inability of the present theory to evaluate the core contributions to $(\tilde{\Lambda})_{\mathfrak{L}}$. In contrast, the deviations in the $^1\Sigma_{sp}$ curves result primarily from the inability of the scattering theory of I to calculate accurate singlet *s*-wave phase shifts, as measured by the disagreement with the variational phase shifts obtained by Geltman[12] and Schwartz[13]. Since this partial wave is the only one that has an orthogonalizing λ term,[15] it is suggested that this method of forcing orthogonalization may provide the dominant limitation on the scattering theory of I. In addition, some of the noticeably larger disagreement between $(\tilde{\Lambda})_{\mathfrak{L}}$ and $(\tilde{\Lambda})_{\mathfrak{V}}$ at the higher initial electron energies must be due to the limitations of the static polarizability concept at such energies.

The bremsstrahlung cross section was calculated for neutral oxygen using the above technique at a few representative energies. Good agreement was obtained with the full numerical evaluation of the cross section given in I.

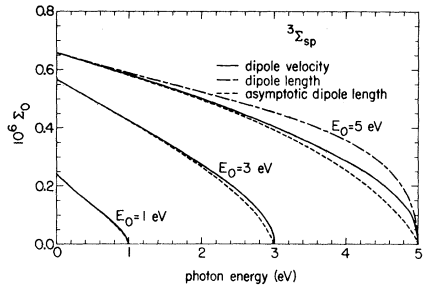

FIG. 3. Σ_0 for triplet *sp* transitions.

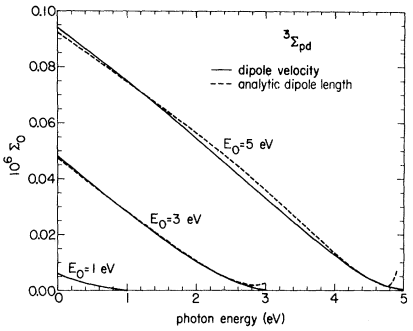

FIG. 5. Σ_0 for triplet *pd* transitions.

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