PHYSICAL REVIEW VOLUME 154, NUMBER 1 5 FEBRUARY 1967

Bremsstrahlung Emission from Low-Energy Electrons on Atoms*

R. C. Mjolsness and Hans M. Ruppel
University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico

(Received 6 July 1966; revised manuscript received 26 September 1966)

General expressions are given for the bremsstrahlung cross section resulting from electron–neutral-atom collisions at energies comparable to or lower than the excitation energies of the atom and for the bremsstrahlung emission from an electron–neutral-atom gas. These quantities have been evaluated for oxygen and nitrogen, and appear to be consistent with shock-tube data. Electron scattering is treated by Hartree-Fock equations which contain neutral-atom bound orbitals and a semiempirical polarization potential. Elastic-scattering data are fitted by the adjustment of a single parameter in the polarization potential. The bremsstrahlung cross section is derived from a distorted-wave theory. The dipole-acceleration form of the matrix element is used for numerical convenience. Because each angular-momentum state has different direct and exchange potentials, the conventional bremsstrahlung formula must be generalized. Approximate analytical expressions for the bremsstrahlung cross section are also obtained from the dipole-length form of the matrix element. From two sorts of resonance phenomena exhibited by the bremsstrahlung cross section—one associated with maxima and minima in the elastic scattering, and one with the relative proportion of *p*-wave to *s*-wave scattering—it may be concluded that an accurate treatment of the electron scattering is necessary for the reliable prediction of bremsstrahlung.

I. INTRODUCTION

NEUTRAL bremsstrahlung and inverse bremsstrahlung are major contributors to emission and absorption processes in a weakly ionized gas. Cases in which these processes are significant typically involve gas temperatures of several thousand degrees Kelvin and include stellar atmospheres,[1] possibly gaseous nebulae, strong shock waves (notably in shock tubes[2]), and the initiation of gaseous breakdown by lasers.[3]

For electron energies comparable to or lower than atomic excitation energies, bremsstrahlung emission is strongly dependent on the details of the electron-atom interaction, and the theoretical description of the emission is not highly developed. A theory is given here for energies of several eV or less in which the electron is assumed to make direct and exchange interactions with the atomic charge cloud via undistorted atomic orbitals in Hartree-Fock equations. A semiempirical polarization potential has been added to account for distortion of the orbitals and to compensate for other approximations in the treatment of the scattering. At higher energies it is necessary to give a different treatment of the electron-atom interaction.

Previously published work on neutral bremsstrahlung includes measurements of gas emissivities,[2,4] analytical[5] and numerical[6–8] treatments of model potentials, and general approximations[9–11] relating the bremsstrahlung cross section to the elastic scattering. In particular, Ohmura and Ohmura[9] develop an analytic expression for the cross section in terms of the *s*-wave elastic-scattering phase shift, while Kas'yanov and Starostin[10] express the cross section in terms of an integral over the differential cross section for elastic scattering.

The results obtained here represent a natural generalization of the Ohmura-Ohmura formula and a somewhat less straightforward generalization of the Kas'yanov and Starostin expression. Specifically, an approximation to the dipole length form of the present theory leads to an analytic expression for the cross section involving the *s*- and *p*-wave phase shifts that appear in the theory, each state of total orbital and spin angular momentum having its own set of phase shifts. This expression reduces to the Ohmura-Ohmura formula when the *p*-wave phase shifts are set equal to zero and the angular momentum of the atom is ignored. In the limit in which the photon energy is much less than the initial electron energy, the Kas'yanov and Starostin expression is proportional to the total momentum transfer cross section. The analytic approximation obtained here is, in the same limit, proportional to the leading term in an angular-momentum decomposition of the momentum transfer cross section. In the Kas'yanov and Starostin work, the treatment is based on consistently ignoring momentum dependences in the elastic-scattering amplitude. The present work puts in such dependences using a model which is an idealization of the actual scattering process but which is brought as close as possible to experiment by adjusting a single parameter.

---

* Work performed under the auspices of the U. S. Atomic Energy Commission.

[1] See, for example, S. Geltman, Astrophys. J. **141**, 376 (1965) and references cited therein.

[2] R. L. Taylor, J. Chem. Phys. **39**, 2354 (1963).

[3] This process has recently been considered both experimentally and theoretically. Results are perhaps typified by J. M. Dawson, Phys. Fluids **7**, 981 (1964).

[4] G. Boldt, Z. Physik **154**, 319 (1959); **154**, 330 (1959).

[5] L. Nedelsky, Phys. Rev. **42**, 641 (1932).

[6] R. V. De Vore, Phys. Rev. **136**, A666 (1964); **140**, AB3 (1965).

[7] R. G. Breene, Jr., and M. Nardone, J. Opt. Soc. Am. **53**, 924 (1963).

[8] M. Ashkin, Phys. Rev. **141**, 41 (1966).

[9] T. Ohmura and H. Ohmura, Astrophys. J. **131**, 8 (1960).

[10] V. Kas'yanov and A. Starostin, Zh. Eksperim. i Teor. Fiz. **48**, 295 (1965) [English transl.: Soviet Phys.—JETP **21**, 193 (1965)].

[11] R. L. Taylor and B. Kivel, J. Quant. Spectry. Radiative Transfer **4**, 239 (1964).

The bremsstrahlung cross section is sensitive not only to the total elastic scattering but also to the ratios of the p-wave to s-wave scattering. Potential scattering models are unlikely to yield this much detail correctly, and have not given accurate values even for the total elastic scattering.[12,13] Thus it is appropriate to introduce the complications of a Hartree-Fock type of approach into the treatment of the electron scattering.

In Sec. II a perturbation theory of the electron-atom scattering is given in which the zeroth-order wave function ϕ_0 describes elastic scattering while ϕ_1 describes one-photon emission. Other inelastic processes are ignored. A method for evaluating ϕ_0 is given and a distorted wave theory is developed for evaluating the asymptotic form of ϕ_1. In Sec. III general expressions for the bremsstrahlung cross section and a number of useful approximations to these expressions are given. In Sec. IV the expression for the emissivity of an optically thin gas is noted. Finally, in Sec. V detailed numerical results are given for oxygen and nitrogen.

II. DESCRIPTION OF ELECTRON-ATOM SCATTERING

A. Atomic States

In the present treatment of electron-atom scattering it is assumed that the atom remains in its ground state during the course of the scattering and that polarization effects are adequately described by a central potential acting on the free electron only. The ground-state atomic wave functions are assumed to be linear combinations of determinantal wave functions, the linear combinations chosen so as to produce eigenfunctions of L^2, S^2, L_z, and S_z. The determinants are to be constructed as usual from one-particle wave functions, and it will be assumed that the same set of radial orbitals is used in each determinant, while the angular and spin parts of the wave functions vary among the determinants. The mathematical description of such systems is by now fairly standard.[14] However, it is desired to present the basic equations of the theory in explicit notation in which the numerous quantum numbers are specified in detail. Much of the notation is defined in this subsection and the following.

Quantum numbers $\alpha=\{n,l,m^l,m^s\}$ for individual bound orbitals, are introduced; the collections of N sets of α's used in a determinantal wave function are denoted by γ. The spatial and spin coordinates of the electrons are denoted by $y_i=\{\mathbf{r}_i,\sigma_i\}$, $i=1,\cdots N+1$, where N electrons are bound and one is free. To facilitate the construction of antisymmetric wave functions, a $4N$-dimensional space is introduced having $3N$ continuous dimensions and N discrete ones. In this space, the wave function is just a number at each point, and explicit antisymmetrization is secured by taking the wave function to be a determinant composed of one-particle orbitals. To perform coordinate integrations in the space it is useful to denote

$$\int dy_i\equiv\int d^3r_i\sum_{\sigma_i}\quad\text{and}\quad\int d\hat{y}_i\equiv\prod_{\substack{j=1\\ j\neq i}}^{N+1}\int dy_j\,,$$

while coordinate integrations in the full $(4N+4)$-dimensional space of the scattering problem are denoted by

$$\int dy\equiv\prod_{j=1}^{N+1}\int dy_j\,.$$

Ground-state wave functions which are eigenfunctions of L^2, S^2, L_z, and S_z will have the form

$$W_{l_2s_2}{}^{m^l,m^s}(\hat{y}_i)=\sum_{\gamma}C_{\gamma}{}^{m^lm^s}D_{\gamma}(\hat{y}_i)\,,\tag{1}$$

where

$$\sum_{\gamma}|C_{\gamma}{}^{m^lm^s}|^2=1\,,$$

$D_\gamma(\hat{y}_i)$ is a Slater determinant, and the $W_{l_2s_2}{}^{m^l,m^s}$ satisfy the usual orthonormality conditions.

The subscripts 2 on the quantum numbers of L^2 and S^2 are introduced for later convenience in the scattering problem in which the free electron (system 1) interacts with the atom (system 2). The $C_\gamma{}^{m^lm^s}$ are readily computed by the methods of Slater,[15] when the relevant configurations are not degenerate, but their specific values are not needed in the remainder of the paper. In an assemblage of ground-state atoms, all values of m^l and m^s will occur, but it seems preferable to work with the $W_{l_2s_2}{}^{m^l,m^s}$ and sum partial cross sections over m^l and m^s rather than to work with incoherent sums of the $W_{l_2s_2}{}^{m^l,m^s}$.

B. States of the Scattering System

In order to obtain uncoupled equations for the various partial waves of the free electron, it is necessary to make approximations to the Hartree-Fock equations for the free orbitals. Fewer approximations are made by choosing the partial waves to be eigenstates of the total L^2, S^2, L_z, and S_z operators of the entire system. The resulting equations then have couplings only among the possible values for the orbital angular momentum of the free electron and these couplings are ignored.

The wave functions $\phi_0(\mathbf{k}_0,y)_{m^lm^s}$ describing the elastic scattering of the system have incoming part

$$\phi_0{}^{in}(\mathbf{k}_0,y)_{m^lm_2{}^s}=A_i\left[\frac{e^{i\mathbf{k}_0\cdot\mathbf{r}_i}}{(2\pi)^{3/2}}\delta(\sigma_i,m_1{}^s)W_{l_2s_2}{}^{m^l,m_2{}^s}(\hat{y}_i)\right],\tag{2}$$

with

$$A_i=\sum_{i=1}^{N+1}\frac{(-1)^{N+1-i}}{(N+1)^{1/2}}\,.$$

---

[12] M. M. Klein and K. A. Brueckner, Phys. Rev. **111**, 1115 (1958).

[13] J. Cooper and J. Martin, Phys. Rev. **126**, 1482 (1962).

[14] M. J. Seaton, Proc. Roy. Soc. (London) **245A**, 469 (1953).

[15] J. C. Slater, Phys. Rev. **34**, 1293 (1929).

The axis of quantization for the angular functions in the bound orbitals is chosen to be $\hat{k}_0$, the direction of the incoming wave. The functions take the form

$$\phi_0(\mathbf{k}_0,y)_{m^l m_2^s}=A_i\sum_L\sum_S\sum_{l_1}(l_1l_2L\,|\,0m^l)(\tfrac{1}{2}s_2S\,|\,m_1^s m_2^s)\times[R_{l_1}{}^{LS}(k_0r_i)/r_i]G_{LSl_1}{}^{m^l,m_1^s+m_2^s}(\hat{\mathcal{Y}}_i)\,,\quad(3)$$

where ϕ_0 has been represented in terms of the eigenfunctions

$$G_{LSl_1}{}^{m^l,m^s}(\hat{\mathcal{Y}}_i)=\sum_{m_1}\sum_{m_2}(l_1l_2L\,|\,m^l-m_1,\,m_1)(\tfrac{1}{2}s_2S\,|\,m^s-m_2,\,m_2)\times Y_{l_1}{}^{m^l-m_1}(\hat{r}_i,\hat{k}_0)\delta(\sigma_i,\,m^s-m_2)W_{l_2s_2}{}^{m_1,m_2}(\hat{\mathcal{Y}}_i)\quad(3\text{a})$$

of angular-momentum operators for the scattering system and the free radial orbitals $R_{l_1}{}^{LS}(kr_i)/r_i$ having the asymptotic form

$$\lim_{r_i\to\infty}\frac{R_{l_1}{}^{LS}(kr_i)}{r_i}=\frac{i^{l_1}}{\pi kr_i}\left(\frac{2l_1+1}{2}\right)^{1/2}\times\exp i\delta_{l_1}{}^{LS}\sin(kr_i-\tfrac{1}{2}l_1\pi+\delta_{l_1}{}^{LS})\,.$$

In the present work, $(l_1l_2j\,|\,m_1m_2)$ represent vector coupling coefficients.[16] The free orbitals $R_{l_1}{}^{LS}$ are to be distinguished from the bound orbitals $R_{n_jl_j}$. The latter appear in the bound wave functions only and are orthonormal.

The radial functions $R_{l_1}{}^{LS}$ are determined from approximations to the Hartree-Fock equations,

$$\int d\hat{\mathcal{Y}}_i\int d\Omega_i\sum_{\sigma_i}G^*{}_{L'S'l_1'}{}^{m^l,m^s}(\hat{\mathcal{Y}}_i)\times\left[H_0-E_A-\frac{\hbar^2k_0{}^2}{2m}\right]\phi_0(\mathbf{k}_0,y)_{m^lm^s}=0\,,\quad(4)$$

where E_A is the Hartree-Fock energy of the atom,

$$H_0=\sum_{i=1}^{N+1}T_i+\sum_{1\le i<j}^{N+1}V_{ij}\,,$$

$$T_i=-(\hbar^2/2m)\nabla_i{}^2-(Ne^2/r_i)+V_p(r_i)P_i$$

and

$$V_{ij}=e^2/|\mathbf{r}_i-\mathbf{r}_j|\,.$$

Note that T_i is a full one-particle Hamiltonian, not just the kinetic-energy operator. Here V_p is a polarization potential having either the standard[17] form

$$V_p(r)=-\tfrac{1}{2}\alpha e^2/(r^2+r_0{}^2)^2\quad(5)$$

or the second form

$$V_p(r)=-\tfrac{1}{2}\alpha e^2r^4/(r^2+r_0{}^2)^4.\quad(6)$$

P_i is a projection operator acting on the radial orbital for the ith electron and having the eigenvalue 1 if the orbital is free and 0 if the orbital is bound. The second form of the polarization potential is used in the numerical work reported in this paper, as discussed in Sec. IIC. The functions ϕ_0 describe all the possible elastic-scattering states of the electron-atom system. An arbitrary electron beam may be decomposed into plane waves with the wave vector serving as a quantization axis while the atom before scattering is in some one of the states $W_{l_2s_2}{}^{m^l,m_2^s}$. Since only the relative orientation of the electron and atom is of significance for the scattering, it is permissible to choose some fixed value for m_1^s. However, it is necessary to consider all possible values for m^l and m_2^s.

When the phase shifts $\delta_{l_1}{}^{LS}$ are determined by solution of the radial equations, the asymptotic form of the ϕ_0 suffices to determine the elastic scattering. In particular, the cross sections for elastic scattering σ_{el} and momentum transfer σ_m are given by

$$\sigma_{\text{el}}=\left(\frac{4\pi}{k_0{}^2}\right)\sum_{l_1}\sum_S\sum_L\frac{2S+1}{2(2s_2+1)}\frac{2L+1}{(2l_1+1)(2l_2+1)}\times(2l_1+1)\sin^2\delta_{l_1}{}^{LS}\quad(7)$$

and

$$\sigma_m=\left(\frac{4\pi}{k_0{}^2}\right)\sum_{l_1}\sum_S\sum_L\sum_{L'}\frac{2S+1}{2(2s_2+1)}\frac{(2L+1)(2L'+1)}{(2l_2+1)}\times W^2(l_1Ll_1+1L'\,|\,l_21)(l_1+1)\sin^2(\delta_{l_1}{}^{LS}-\delta_{l_1+1}{}^{L'S})\quad(8)$$

where W is a Racah coefficient.[16]

Bremsstrahlung emission is described by functions $\phi_{1i}(k,y)_{m^lm^s}$ which satisfy the equations

$$\left[H_0-E_A-\frac{\hbar^2k^2}{2m}\right]\phi_{1i}(k,y)_{m^lm^s}=-H_{1i}\phi_0(\mathbf{k}_0,y)_{m^lm^s}\quad(9)$$

in the same sense that the functions $\phi_0(\mathbf{k}_0,y)_{m^lm^s}$ satisfy the unperturbed Schrödinger equation defined by H_0. In the above, H_0 and E_A are as defined previously and

$$H_{1i}=-\left(\frac{ie\hbar}{mc}\right)\left(\frac{hc}{k_2\mathcal{V}}\right)^{1/2}\hat{\epsilon}_i\cdot\sum_{j=1}^{N+1}\nabla_j\,,\quad i=1,\,2\,,$$

where $\mathcal{V}$ is a normalization volume for the photon density, $\mathbf{k}_2$ is the photon wave vector, $\hat{\epsilon}_i$ are unit polarization vectors perpendicular to $\mathbf{k}_2$. Of course, both polarizations contribute to the total cross section for bremsstrahlung emission. The physical solutions ϕ_{1i} of Eq. (9) have the asymptotic form

$$\phi_{1i}{}^{\text{asym}}(k,y)_{m^lm^s}=\sum_{m^{l'}}\sum_{m^{s'}}A_j\frac{e^{ikr_j}}{r_j}f_i(\hat{r}_j,\sigma_j\,|\,m^lm^sm^{l'}m^{s'})\times W_{l_2s_2}{}^{m^{l'},m^{s'}}(\hat{\mathcal{Y}}_j)\,,\quad(10)$$

---

[16] M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957). The vector coupling coefficients used in this work have the properties of Rose's $C(l_1l_2j;\,m_1m_2)$ symbols.

[17] M. H. Mittleman and K. M. Watson, Phys. Rev. **113**, 198 (1959); R. A. Buckingham, Proc. Roy. Soc. (London) **A160**, 94 (1937).

corresponding to spherical outgoing waves. Only the asymptotic form of the ϕ_{1i} is needed to determine the bremsstrahlung cross section.

C. Evaluation of ϕ_0 and ϕ_1

When $l_1 \neq l_1'$ terms are dropped from Eq. (4), and the necessary sums and integrations over coordinates are performed, the equation may be brought to the form

$$\left[\frac{\hbar^2}{2m}(\nabla_{l_1'}{}^2+k_0{}^2)-V_{L'S'l_1'}(r)\right][R_{l_1'}{}^{L'S'}(k_0r)/r]$$

$$=\int_0^\infty dr' r'^2 J_{L'S'l_1'}(r,r')[R_{l_1'}{}^{L'S'}(k_0r')/r']$$

$$-\sum_{j=1}^{\hat{N}} \lambda_j{}^{L'S'l_1'}[R_{n_jl_j}(r)/r], \quad (11)$$

where

$$\nabla_{l_1'}{}^2=\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l_1'(l_1'+1)}{r^2},$$

$$V_{L'S'l_1'}(r)=-Ne^2/r+V_p(r)+e^2\sum_{k=0}^{\infty}\sum_{j=1}^{\ddot{N}} a_{kj}{}^{L'S'l_1'}$$

$$\times\int_0^\infty dr'\left(\frac{r_<{}^k}{r_>{}^{k+1}}\right)R_{n_jl_j}{}^2(r'),$$

$$J_{L'S'l_1'}(r,r')=e^2\sum_{k=0}^{\infty}\sum_{j=1}^{\hat{N}} b_{kj}{}^{L'S'l_1'}$$

$$\times\left(\frac{r_<{}^k}{r_>{}^{k+1}}\right)\frac{R_{n_jl_j}(r)}{r}\frac{R_{n_jl_j}(r')}{r'}.$$

$\hat{N}$ is the number of independent pairs of quantum numbers n_jl_j, and $r_<(r_>)$ is the smaller (larger) of r and r'. The constants $\lambda_j{}^{L'S'l_1'}$ are chosen so as to enforce orthogonality between the free and the bound orbitals when the orthogonality is not guaranteed by the angular parts of the functions. Otherwise $\lambda_j{}^{L'S'l_1'}$ is zero. The constants $a_{kj}{}^{L'S'l_1'}$ and $b_{kj}{}^{L'S'l_1'}$ may be found by a formal application of Slater's[15] method for finding electrostatic energies of an atom. Appropriate diagonal matrix elements of H_0 are formed and differentiated functionally with respect to the free orbital. After functional differentiation, all quantities become finite and Eq. (11) is obtained. The advantage of the method is that it is not necessary to construct $G_{L'S'l_1'}{}^{m^l,m^s}$ directly. In case of degeneracy the procedure is made definite by retaining only terms arising from the ground state of the atom in forming the diagonal matrix elements. The coefficients $a_{kj}{}^{L'S'l_1'}$ and $b_{kj}{}^{L'S'l_1'}$ may be obtained by inspection either before or after functional differentiation of the appropriate matrix elements.

The form of the polarization potential of Eq. (6) has been used in all the numerical work reported here. The polarization potential as used here serves to compensate for approximations made in the treatment of the scattering: the neglect of various configurations of the atom in setting up Hartree-Fock equations, the neglect of couplings in these equations, and the use of undistorted atomic orbitals in the equations for the free orbitals. Thus the polarization potential typically has to compensate for both polarization and correlation effects. The form of the polarization potential used here is much closer to the Bauer and Brown[18] expression for a correlation potential at intermediate distances of $\frac{1}{2}$ to several Bohr radii than is the standard form. In the standard form of the potential, a variational calculation yields an expression for r_0 in terms of α.[17] Frequently the use of the semiempirical potential involves varying α while maintaining the connection between r_0 and α. Here the procedure is to hold α fixed while varying r_0. The justification for the latter is that α is an experimental number, typically known to within 15%. Moreover, in view of the number of the effects for which the potential is required to compensate, neither the mathematical form of the cutoff nor the relation between r_0 and α can be regarded as given *a priori*. In fitting elastic-scattering cross sections numerically, it has been found that the uncertainty in the measured values of α may be compensated for by small changes in r_0.

The values of $\lambda_j{}^{L'S'l_1'}$ are in general determined variationally. However, the numerical work reported here has been done with all $\lambda_j{}^{L'S'l_1'}$ equal to zero. For test cases this has resulted in little error, since the values of λ necessary to secure proper orthogonality were small.

Only the asymptotic form of ϕ_1 is needed for the evaluation of bremsstrahlung. This simplifies the application of Green's-function techniques for the determination of the scattering amplitude f_i. This calculation is outlined in Appendix A and yields

$$f_i(\mathbf{r},\sigma\,|\,m^lm^s,m^{l'}m^{s'})=8\pi^2 i\left(\frac{\alpha}{3k_2\mathcal{V}}\right)^{1/2}\sum_{LL'}\sum_{S}\sum_{l_1l_1'}\sum_{M}\sum_{m}(\tfrac{1}{2}s_2S\,|\,m_1{}^sm^s)(\tfrac{1}{2}s_2S\,|\,m_1{}^s+m^s-m^{s'},\,m^{s'})$$

$$\times(l_1'l_2L'\,|\,M-m^{l'},\,m^{l'})(l_1l_2L\,|\,0m^l)(l_11l_1'\,|\,m^l-m,\,M-m^l)(l_1'l_2L'\,|\,M-m,\,m)(l_1l_2L\,|\,m^l-m,\,m)$$

$$\times i^{2l_1'}[(l_1+1)^{1/2}\delta(l_1',\,l_1+1)-l_1{}^{1/2}\delta(l_1',\,l_1-1)]\frac{\Lambda_{LSl_1}{}^{L'S'l_1'}}{(2l_1'+1)}\delta(\sigma,\,m_1{}^s+m^s-m^{s'})Y_{l_1}{}^{M-m^{l'}}(\hat{r},\hat{k}_0)Y^*{}_1{}^{M-m^l}(\hat{\epsilon}_i,\hat{k}_0), \quad (12)$$

---

[18] E. Bauer and H. N. Browne, *Atomic Collision Processes*, edited by M. R. C. McDowell (North-Holland Publishing Company, Amsterdam, 1964), p. 16.

where

$$\Lambda_{LSl_1}{}^{L'Sl_1'}=\int_0^\infty rdr\, R_{l_1'}{}^{L'S}(kr)\left[\frac{d}{dr}+\frac{a_{l_1,l_1'}}{r}\right]\frac{R_{l_1}{}^{LS}(k_0r)}{r} \tag{13}$$

with

$$a_{l_1,l_1+1}\equiv -l_1 \quad\text{and}\quad a_{l_1,l_1-1}\equiv (l_1+1).$$

From Eq. (12) it is readily seen that the scattering amplitudes for bremsstrahlung may be determined algebraically when the radial wave functions for electron-atom elastic scattering are known.

III. BREMSSTRAHLUNG CROSS SECTION

The bremsstrahlung cross section may be obtained from the expression

$$\sigma=\frac{1}{(2l_2+1)}\frac{(2\pi)^3}{(2s_2+1)}\left(\frac{k}{k_0}\right)\sum_{m^l,m^{l'}}\sum_{m^s,m^{s'}}\sum_i\sum_\sigma\int d\Omega\int d\Omega_{\epsilon_i}\left(\frac{\mathcal{V}k_2{}^2}{8\pi^3\hbar c}\right)|f_i(\mathbf{r},\sigma|m^lm^sm^{l'}m^{s'})|^2 \tag{14}$$

in which electron and photon statistical weights have been included. The expressions for the cross section and the scattering amplitude contain all necessary summations and integrations over particle coordinates and channel indices. The symbol $\int d\Omega_{\epsilon_i}$ denotes an integration over all directions of the photon polarization vector $\hat{\epsilon}_i$.

It is convenient to have expressions for the cross section in which the matrix elements are specifically in dimensionless form. To achieve this, all quantities are expressed in atomic units and the free orbitals are normalized according to the more usual convention

$$\lim_{r\to\infty} R_{l_1}{}^{LS}(kr)=\frac{1}{k}\sin(kr-\tfrac{1}{2}l_1\pi+\delta_{l_1}{}^{LS}).$$

Then Eq. (14) takes the form

$$\sigma=\Sigma_0(\pi a_0{}^2/\hbar k_2c), \tag{15}$$

where

$$\Sigma_0=\left(\frac{8}{3\pi}\right)\alpha^3\frac{k}{k_0}\sum_{l_1,l_1'}\sum_S\sum_{L,L'}\frac{2S+1}{2(2s_2+1)}\frac{(2L+1)(2L'+1)}{(2l_2+1)}W^2(l_1'L'l_1L|l_21)$$
$$\times[(l_1+1)\delta(l_1',l_1+1)+l_1\delta(l_1',l_1-1)]|\tilde{\Lambda}_{LSl_1}{}^{L'Sl_1'}|^2, \tag{16}$$

α is the fine structure constant, and a_0 is the Bohr radius. In the above, $\tilde{\Lambda}_{LSl_1}{}^{L'Sl_1'}$ is proportional to $\Lambda_{LSl_1}{}^{L'Sl_1'}$ of Eq. (13). However, $\Lambda_{LSl_1}{}^{L'Sl_1'}$ is formally divergent because of the continuum normalization of the free orbitals. This difficulty may be removed by carrying through a wave-packet analysis of the scattering problem. This results in a convergence factor being inserted in the defining expression for the matrix element. However, it is frequently more useful, for numerical evaluation of the matrix element, to employ the dipole acceleration form

$$\begin{aligned}\Lambda_{LSl_1}{}^{L'Sl_1'}&\equiv\tilde{\Lambda}_{LSl_1}{}^{L'Sl_1'}(k_0{}^2-k^2)^{-1}\\
&=\frac{2m}{\hbar^2}(k_0{}^2-k^2)^{-1}\int_0^\infty rdr\Bigg[R_{l'}{}^{L'S}(kr)\left(\frac{d}{dr}+\frac{a_{l_1,l_1'}}{r}\right)\Bigg(V_{LSl_1}(r)\frac{R_{l_1}{}^{LS}(k_0r)}{r}\\
&\quad-\sum_{j=1}^{\hat{N}}\lambda_j{}^{LSl_1}R_{n_jl_j}(r)+\int_0^\infty dr'r'J_{LSl_1}(r,r')R_{l_1}{}^{LS}(k_0r')\Bigg)+R_{l_1}{}^{LS}(k_0r)\left(\frac{d}{dr}+\frac{[2-a_{l_1,l_1'}]}{r}\right)\\
&\quad\times\left(V_{L'Sl_1'}(r)\frac{R_{l_1'}{}^{L'S}(kr)}{r}-\sum_{j=1}^{\hat{N}}\lambda_j{}^{L'Sl_1'}R_{n_jl_j}(r)+\int_0^\infty dr'r'J_{L'Sl_1'}(r,r')R_{l_1'}{}^{L'S}(kr')\right)\Bigg]\end{aligned} \tag{17}$$

which is obtained from Eq. (13) by use of Eq. (11) for the free orbitals and by integration by parts. In the above expression all integrals are convergent. The $\tilde{\Lambda}_{LSl_1}{}^{L'Sl_1'}$ of Eq. (16) for Σ_0 is defined by Eq. (17).

In applications of the above formalism, sufficient accuracy may be obtained by neglecting the $L(L')$ dependence of the matrix element when $l_1>l_1'$ $(l_1'>l_1)$. In this approximation, Eq. (16) simplifies to

$$\Sigma_0=\left(\frac{8}{3\pi}\right)\alpha^3\frac{k}{k_0}\sum_{l_1}\sum_S\sum_L\frac{2S+1}{2(2s_2+1)}\frac{2L+1}{(2l_1+1)(2l_2+1)}(l_1+1)(|\tilde{\Lambda}_{LSl_1}{}^{LSl_1+1}|^2+|\tilde{\Lambda}_{LSl_1+1}{}^{LSl_1}|^2). \tag{18}$$

This form of Σ_0 is used to produce the numerical results for σ reported below.

It is possible to obtain a direct generalization of the Ohmura-Ohmura formula[9] by making use of the dipole length form of the matrix element which in atomic units becomes

$$\Lambda_{LSl_1}{}^{L'Sl_1'}=\tfrac{1}{2}(k_0^2-k^2)\int_0^\infty dr\, e^{-\epsilon r}rR_{l_1'}{}^{L'S}(kr)R_{l_1}{}^{LS}(k_0r)\,, \tag{19}$$

and in which the necessary convergence factor has been inserted explicitly. This expression for the matrix element is not exact, since the quantities $\phi_0(\mathbf{k}_0,y)_{m^lm^s}$ are not really eigenfunctions of H_0, and it differs from the expression of Eq. (17) by certain integral terms which will be ignored here. When l_1 and l_1' have the values zero and 1, a useful approximation to Eq (19) is obtained by assuming that

$$R_l{}^{LS}(kr)/r=\cos\delta_l{}^{LS}j_l(kr)-\sin\delta_l{}^{LS}n_l(kr)\,,\quad \text{for}\quad l=0,1. \tag{20}$$

This approximation is not useful for higher l values, however, and no useful extension of Eq. (20) to such values has been found. Thus, it is necessary to assume that l_1, $l_1'>1$ are of negligible importance to the bremsstrahlung cross section if this approximation is to be used to evaluate σ. With the above approximations an equation analogous to Eq. (16) may be derived and is given by

$$\Sigma_0=\left(\frac{2}{3\pi}\right)\frac{\alpha^3}{kk_0^3}\sum_{l_1,l_1'}\sum_S\sum_{L,L'}\frac{2S+1}{2(2s_2+1)}\frac{(2L+1)(2L'+1)}{(2l_2+1)}W^2(l_1'L'l_1L|l_21)$$
$$\times\Bigg[\delta(l_1,0)\delta(l_1',1)\left\{\frac{k_0}{k}(k_0^2-3k^2)\cos\delta_0{}^{LS}(k_0)\sin\delta_1{}^{LS}(k)+2k^2\sin\delta_0{}^{LS}(k_0)\cos\delta_1{}^{LS}(k)\right\}^2$$
$$+\delta(l_1',0)\delta(l_1,1)\left\{\frac{k}{k_0}(k^2-3k_0^2)\cos\delta_0{}^{LS}(k)\sin\delta_1{}^{LS}(k_0)+2k_0^2\sin\delta_0{}^{LS}(k)\cos\delta_1{}^{LS}(k_0)\right\}^2\Bigg]. \tag{21}$$

An expression analogous to Eq. (18) is readily obtained by neglecting the $L(L')$ dependence of Eq. (21).

In the cases considered numerically, the neglect of higher l_1 and l_1' values in these equations leads to as much as a 20% error in σ. Of course neglect of all L and S dependences of the matrix elements in Eq. (18) yields the corresponding potential scattering formula. The above expressions for Σ_0 reduce to the Ohmura-Ohmura formula[9] when all $\delta_l{}^{LS}$ are taken to be zero. It may be verified from Eq. (21) that Σ_0 is proportional to the leading term of Eq. (8) for σ_m when $k\rightarrow k_0$, with the constant of proportionality given by Eq. (25). It would appear that the present theory also forms a generalization of the Kas'yanov-Starostin result,[10] since these authors obtain in the same limit Σ_0 proportional to σ_m, with the same constant of proportionality. Presumably, a more accurate treatment of Eq. (19) for higher orbital angular momenta would confirm the full proportionality.

IV. BREMSSTRAHLUNG EMISSION FROM AN OPTICALLY THIN GAS

A quantity of frequent observational interest is the volume emission coefficient of an optically thin gas. Expressions in which transitions between zero-photon and one-photon states only are evaluated are given below for the bremsstrahlung contributions to this emissivity. The gas is assumed to consist of electrons of temperature T and density n and a single species of atoms of density N in the ground state, although the formulas given may readily be generalized to include more species of atoms. However, molecules, atoms in excited states, and ions are not considered. This neglect is often justified when neutral bremsstrahlung is a dominant process. To include the contributions from other species it is necessary to calculate Σ_0 appropriately. The calculation has already been done for ions in the Coulombic approximation. When neutral bremsstrahlung is the predominant emission mechanism, it is usually permissible to set N equal to the total atom density.

The total volume emission coefficient J is given by

$$J=\frac{Nn}{4\pi}\int d^3v\, vf(v)\int d(\hbar ck_2)\hbar ck_2\sigma\,, \tag{22}$$

where the electron distribution function

$$f(v)=(m/2\pi kT)^{3/2}\exp[-\tfrac{1}{2}(mv^2/kT)]\,,$$

σ is the bremsstrahlung cross section computed above, and all photon wave numbers are integrated. To compare with experiment, it is convenient to have an expression for the emission per unit wavelength. Use of Eq. (22) and the relation $J=\int d\lambda_\mu J(\lambda_\mu)$, where λ_μ is the photon wavelength in microns, leads to

$$J(\lambda_\mu)=1.204\times10^{-25}Nn\theta^{3/2}\lambda_\mu{}^{-2}$$
$$\times\int_{k_0^2=\Delta k^2}^\infty dk_0k_0^3e^{-31.33\theta k_0^2}\Sigma_0\ \mathrm{W/cm^3}\ \mu\ \mathrm{sr}\,, \tag{23}$$

TABLE I. The coefficients $a_{kj}^{LSl_1}$ and $b_{kj}^{LSl_1}$ (the latter in parentheses) used in the radial wave equations. In the case of the degenerate ^2P and ^2D states for oxygen and ^3P for nitrogen, only those coefficients which relate to the ground state are tabulated.

		Oxygen									Nitrogen				
		$L=1, l_1=0$		$L=0, l_1=1$		$L=1, l_1=1$		$L=2, l_1=1$			$L=0, l_1=0$		$L=1, l_1=1$		
n_jl_j	$S \backslash k$	0	1	0	2	0	2	0	2	$S \backslash k$	0	1	0	1	2
$1s$	1/2	2 (−1)		2 (−1/3)		2 (−1/3)		2 (−1/3)		1	2 (−1)		2	(−1/3)	
	3/2	2 (−1)		2 (−1/3)		2 (−1/3)		2 (−1/3)		2	2 (−1)		2	(−1/3)	
$2s$	1/2	2 (−1)		2 (−1/3)		2 (−1/3)		2 (−1/3)		1	2 (−1)		2	(−1/3)	
	3/2	2 (−1)		2 (−1/3)		2 (−1/3)		2 (−1/3)		2	2 (−1)		2	(−1/3)	
$2p$	1/2	4		4 (−1)	10/25 (−10/25)	4 (2)	−5/25 (−5/50)	4 (−1)	1/25 (7/50)	1	3	(1/3)	3 (1/3)		(2/15)
	3/2	4	(−1)	4 (−1)	10/25 (−10/25)	4 (−1)	−5/25 (−10/25)	4 (−1)	1/25 (−10/25)	2	3	(−1)	3 (−1)		(−10/25)

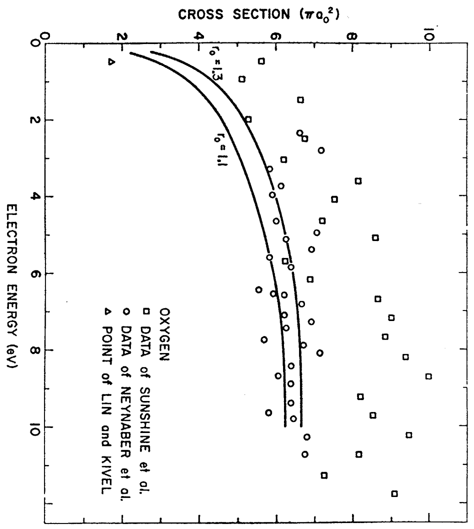

FIG. 1. Elastic-scattering cross section of electrons on oxygen. Theoretical curves have r_0 of 1.1 and 1.3 a.u. Data points of Sunshine *et al.*, Lin and Kivel, and Neynaber *et al.* [R. Neynaber, L. Marino, E. Rothe, and S. Trujillo, Phys. Rev. **123**, 148 (1961); **129**, 2069 (1963)] are given.

where $\theta=5040/T$, the densities are expressed in cm^{-3}, k_0 and k are expressed in inverse Bohr radii, and Σ_0 is given by Eq. (16). In the above integration, $\Delta k^2=k_0^2-k^2$ is kept fixed as k_0 varies.

For oxygen and nitrogen, Σ_0 is well approximated by $\Sigma_0=\sigma_0(k_0^2-\Delta k^2)$. With this assumption $J(\lambda_\mu)$ may be evaluated as

$$J(\lambda_\mu)=2.402\times10^{-31}$$
$$\times\sigma_0 N n\theta^{-7/2}[u+2]u^2e^{-u}\ \mathrm{W/cm^3}\ \mu\ \mathrm{sr} \quad (24)$$

where $u\equiv31.33\theta\Delta k^2=2.855\theta\lambda_\mu^{-1}$. The expression of Eq. (24) is convenient for comparison with experimental data but does not have general validity. In general, $J(\lambda_\mu)$ must be evaluated numerically.

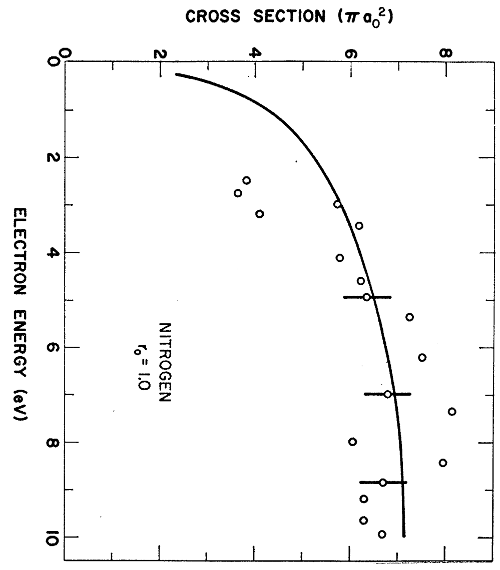

FIG. 2. Elastic-scattering cross section of electrons on nitrogen. The theoretical curve with $r_0=1.0$ a.u. is compared with the data of Neynaber *et al.* [R. Neynaber, L. Marino, E. Rothe, and S. Trujillo, Phys. Rev. **123**, 148 (1961); **129**, 2069 (1963)].

V. NUMERICAL RESULTS FOR NITROGEN AND OXYGEN

A. Elastic-Scattering Cross Sections

The key to the evaluation of the bremsstrahlung cross section is the calculation of accurate radial functions for the partial waves of the free electrons. The equation for each partial wave has the form of an uncoupled, second-order integrodifferential equation. Inputs for these calculations are values of the polarizability α, the adjustable parameter r_0, and the coefficients $a_{kj}{}^{LSl_1}$ and $b_{kj}{}^{LSl_1}$. The polarizability is obtained from experiment, though theoretical values also exist. The coefficients $a_{kj}{}^{LSl_1}$ and $b_{kj}{}^{LSl_1}$ are obtained by formal application of Slater's method[15] and are collected for convenience in Table I. The parameter r_0 is determined by a fit to the elastic-scattering cross section data.

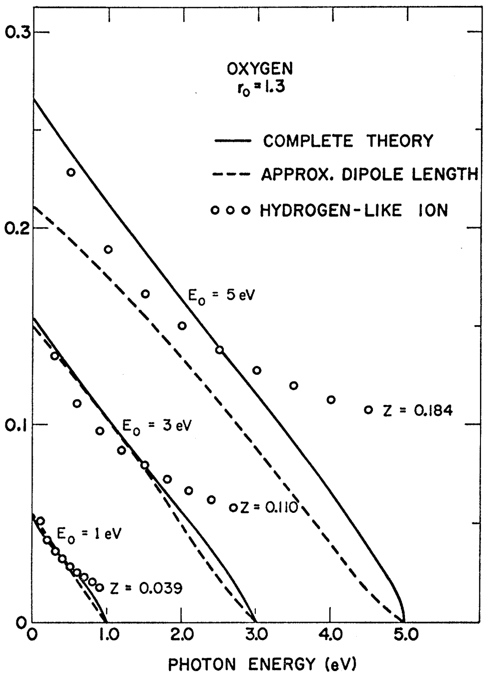

FIG. 3. Calculated values of Σ_0 for the bremsstrahlung cross section of electrons on oxygen. Results are given for the full theory and for an analytic approximation to the dipole length matrix elements. The circles represent the Elwert approximation to the bremsstrahlung from a hydrogen-like ion. For each initial electron energy, a separate z was needed.

The integrodifferential equation for the radial functions is solved by iteration. The nth iterate of Eq. (12) may be written symbolically as

$$H(r)[R_{l_1'}{}^{L'S'}(k_0r)/r]_n = 2Q_n(r)/r$$

where

$$Q_n(r) = (1-x)\tilde{Q}_n + xQ_{n-1},$$

in which

$$2\tilde{Q}_n(r)/r = \int_0^\infty dr' r'^2 J_{L'S'l_1'}(r,r') \times \left[\frac{R_{l_1'}{}^{L'S'}(k_0r')}{r'}\right]_{n-1}, \quad \text{for } n>1,$$

and x is a parameter chosen to enforce convergence. At each iteration $[R_{l_1'}{}^{L'S'}(kr)/r]_n$ is obtained from the solution of an inhomogeneous differential equation and

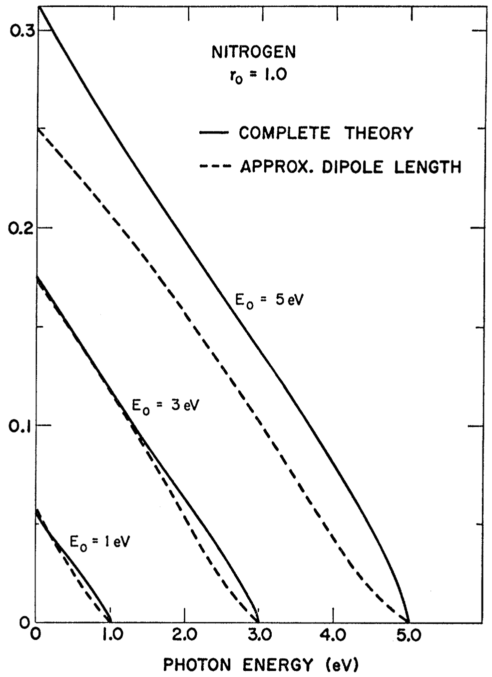

FIG. 4. Calculated values of Σ_0 for electrons on nitrogen. Results are given for the full theory and for an analytic approximation to the dipole length matrix elements.

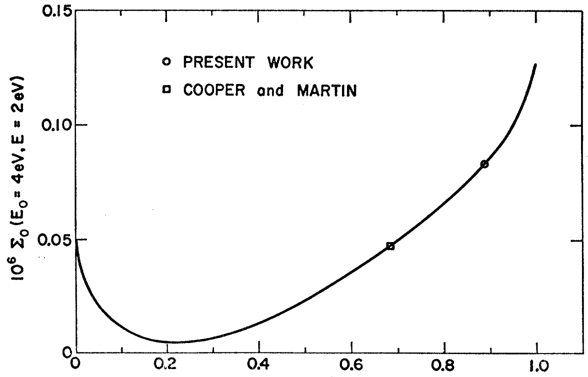

FIG. 5. Dependence of Σ_0 on the ratio of s wave to total elastic scattering for oxygen. The total elastic-scattering cross section is kept fixed at 2 eV and at 4 eV, while the ratios of s-wave to p-wave scattering are varied. Ratios appropriate to the present theory and to the theory of Cooper and Martin are indicated.

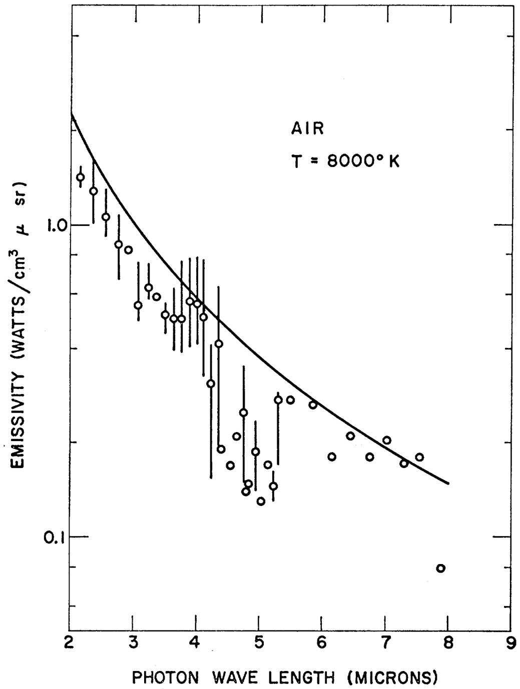

FIG. 6. Calculated and experimental continuum emissivity for air at 8000°K. Experimental points are from the shock tube data of Taylor.

is used to compute $\tilde{Q}_{n+1}$. The process is started by choosing some reasonable values of Q_1 as inputs. Converged values of $R_{l_1'}{}^{L'S'}$ are used to compute the bremsstrahlung matrix elements.

The choice of x merits discussion. For $x=0$ convergence is slow, while in some cases with $x=\frac{1}{2}$ a quasi-convergence occurs in which $[R]_{2n}$ and $[R]_{2n+1}$ converge to different functions having phase shifts π apart. A value $x=0.6$ has been found adequate to provide a rapid and real convergence. Tests of the convergence of the scheme have been made using widely disparate Q_1 values. It is found that convergence to the same $R_{l_1'}{}^{L'S'}$ occurs in every case.

The values chosen for the polarizability in units of $a_0{}^3$ are 5.6 for oxygen and 8.2 for nitrogen, which agree roughly with theoretical calculations and are within the experimental errors of existing measurements.[19] The precise values are not considered to be critical and small changes in α may be compensated for by changes in r_0.

In Figs. 1 and 2 are displayed the fits to the experimental elastic cross section for oxygen ($r_0=1.1$ and 1.3) and nitrogen ($r_0=1.0$). Although the shock tube measurement of Lin and Kivel[20] at approximately 0.5 eV disagrees with the calculated curve, considerable latitude is permitted by present information in the reduction of the Lin and Kivel data. It is consistent with experimental errors to place the Lin and Kivel point anywhere between $1.3\pi a_0{}^2$ and $4.0\pi a_0{}^2$.

The oxygen data of Sunshine *et al.*,[21] lie uniformly higher than the calculated curve. Some efforts have been made to adjust r_0 and α to determine whether reasonable fits to these data are possible. However, it appears that physically unacceptable values of both α and r_0 would be necessary in the present model to attain such large values for the cross section, although a fit to the mean of all the data presumably could be found.

In the case of nitrogen, the calculated curve gives a good fit to the experimental data and for both atomic species the fits were felt to be sufficiently close to justify using the wave functions for calculating the bremsstrahlung.

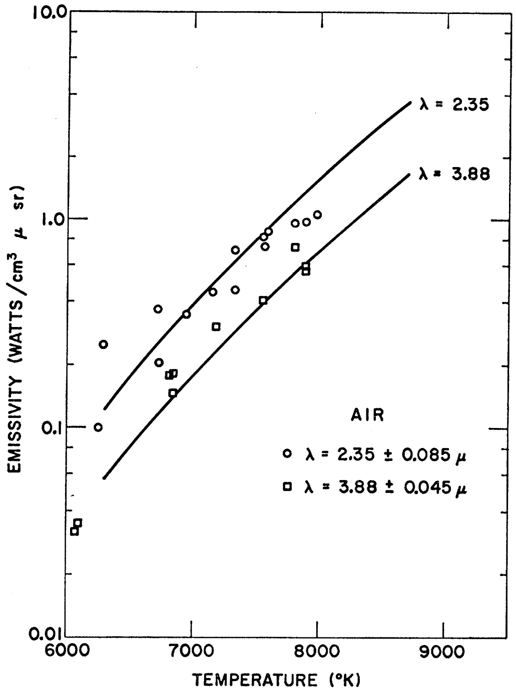

FIG. 7. Temperature dependence of the continuum emissivity of air. Taylor's data are displayed together with the present theoretical results.

B. Bremsstrahlung Cross Section

The radial wave functions, obtained as described in the previous section, are substituted into Eq. (18) and yield the cross section for bremsstrahlung. The results of the calculation are displayed in Figs. 3 and 4 for atomic oxygen and nitrogen, respectively. The solid curves represent the complete calculation in which both *s-p* and *p-d* transitions are included. The *d-f* transition was found to contribute less than 1% in all cases and was omitted.

---

[19] A. Dalgarno, Advan. Phys. **11**, 289 (1962).

[20] S. C. Lin and B. Kivel, Phys. Rev. **114**, 1026 (1959).

[21] G. Sunshine, B. Aubrey, and B. Bederson, in *Proceedings of the Fourth International Conference on the Physics of Electronic and Atomic Collisions, Quebec, 1965*, edited by L. Kerwin and W. Fite (Science Bookcrafters, Inc., Hastings-on-Hudson, New York, 1965).

The dashed curves are calculated from the approximate dipole length formula and contain only *s-p* transitions. Thus, at the higher initial energies where the *p-d* contribution is of the order of 10 to 20%, the dipole length approximation departs significantly from the more exact calculation. However, this approximation agrees within 5 to 7% with the *s-p* contributions of the full calculation in each case.

To examine the approximations to the complete theory, emissivities were calculated for oxygen and nitrogen with the linear form Eq. (24) and the approximate dipole length form and compared to the complete theory. For oxygen $\sigma_0 = 0.71 \times 10^{-6}$ and for nitrogen $\sigma_0 = 0.80 \times 10^{-6}$. Except at the lowest wavelengths, the emissivities are effectively the same in each of the three cases. Hence, it would appear that for the calculation of absorption and emission coefficients the approximate formulations yield results adequate for most purposes.

On Fig. 3 for oxygen, the bremsstrahlung from a Coulomb potential is shown. The Elwert[22] approximation was fitted with an effective z at $E = E_0/2$ for each initial energy. Not only is the fitted z very sensitive to the initial energy, but even for a single electron energy the purely Coulombic bremsstrahlung does not give a satisfactory energy dependence for the cross section. The fitted z contains a strong energy dependence; use of a single z for all E_0 destroys even order of magnitude agreement with the present calculation over some energy ranges. Thus, the use of this approximation to interpret experimental data, as done, for example, by Taylor,[2] is without foundation and may lead to order of magnitude errors.

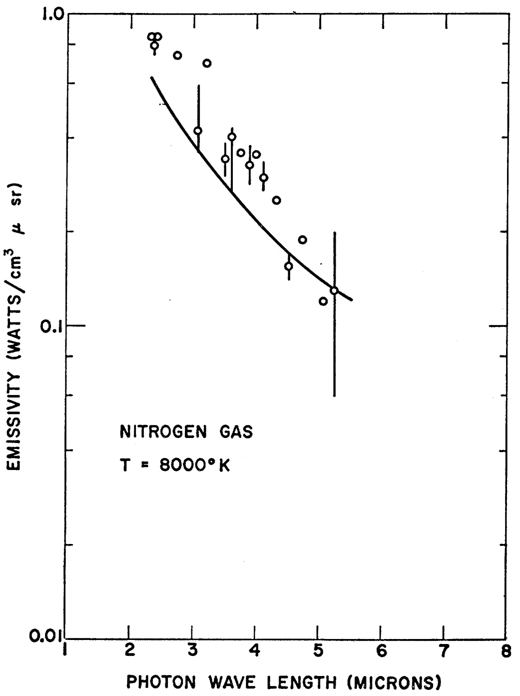

FIG. 8. Calculated and experimental continuum emissivity of nitrogen at 8000°K. Experimental points are from Taylor's data.

Since the elastic cross sections are the only experimental data against which the present model has been tested in detail, it is of interest to examine the sensitivity of the bremsstrahlung cross section to the amount of s wave in the elastic scattering. With the total elastic cross section held fixed, the ratio of s wave to total elastic cross section was allowed to vary and Σ_0 was obtained using the approximate dipole length formulation for *s-p* transitions. The results for oxygen are shown in Fig. 5.

The curve shows an order of magnitude variation in Σ_0. Hence it is apparent that phase shifts which fit the elastic-scattering cross section may not give a correct bremsstrahlung cross section. In particular, a pure potential model of the interaction may yield the elastic data and yet give a poor representation of the bremsstrahlung. For example, the work of De Vore[6] on nitrogen shows order of magnitude differences with the present results at some energies.

The point of Cooper and Martin is included for comparison. It was obtained from the ratio of their 4-eV s wave to their total cross section. The present fit contains relatively less p-wave contribution and is indicated on the graph.

A definitive estimate of the over-all accuracy of the computed bremsstrahlung cross section cannot be given

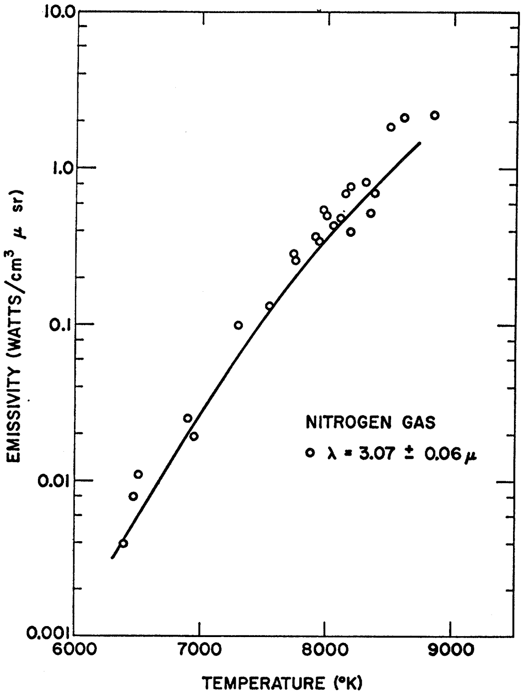

FIG. 9. Temperature dependence of the continuum emissivity of nitrogen. Experimental points are from Taylor's data.

---

[22] J. Greene, Astrophys. J. **130**, 693 (1959).

at present. Almost certainly the approximations made in evaluating the theory of Secs. II and III result in less than a 7% error in Σ_0, as discussed in the following paragraphs.

For oxygen, scattering occurs for p waves in ^4D, ^4P, ^4S, ^2D, ^2P, and ^2S states. The configurations ^2D and ^2P are degenerate, and the entire scattering is assumed to occur in the state with the highest statistical weight, the ^4D state. Scattering for $l=2$ is assumed for simplicity to occur only in a single state in which all exchange terms are ignored. All scattering in free-electron states with $l>2$ is ignored. A similar approximation is made for nitrogen. This shortens the numerical work and avoids a direct treatment of degeneracies. The approximation was tested in a few cases, and it was found that putting in all the L and S dependences according to the rules given in Sec. IIC above lowered Σ_0 by less than 5%. In addition, all Lagrange multipliers were ignored. This omission was justified by a few test cases in which multipliers forcing the proper orthogonality of the orbitals were obtained. The multipliers were small and had little effect on the differential equations.

The uncertainty in the value of r_0 should result in less than an 8 or 9% error. The errors in the theory itself are harder to assess. A number of couplings have been ignored which can in principle yield appreciable discrepancies. At low photon energies, these errors will be manifested through an incorrect calculation of the momentum-transfer cross section. If the spread of points in the total elastic-scattering data may be used as a measure of the uncertainty in the momentum transfer, the error in the bremsstrahlung in the low-photon-energy limit should be less than 40% for oxygen and less than 15% for nitrogen. The larger number for oxygen is due to the extreme spread of the experimental data and is probably a considerable overestimate.

However, the approximations made in solving for the zeroth-order wave function of the system may be tested more directly by comparing values of Σ_0 calculated with the dipole acceleration and dipole length forms of the matrix element, Eqs. (16) and (21), respectively. The two equations are equivalent only when the zeroth-order wave function is a solution of the unperturbed many-particle Schrödinger equation. Therefore, the differences in Σ_0 obtained from these equations should provide an estimate of the uncertainty in Σ_0. It is found that the two calculations agree to within 10% in most cases. Agreement is within 1% in the most favorable cases and within 20% in the worst case, with the larger errors occurring when the final electron energy is much smaller than the initial energy.

C. Calculation of Emissivity

It is possible to combine the above results with an approximate evaluation of bremsstrahlung emission from a nitrogen molecule to obtain emissivities for air and nitrogen gas. To evaluate the electron-molecule contribution to the radiation two approximations are made. It is assumed that the zero-photon-energy limit of the cross section may be used even for photon energies which are an appreciable fraction of the average electron energy; it is also assumed that the correct zero-photon-energy bremsstrahlung is proportional to the momentum-transfer cross section, i.e.,

$$\Sigma_0=(4/3\pi^2)k_0^2\alpha^3\sigma_m. \tag{25}$$

For the nitrogen molecule σ_m given by Engelhardt *et al.*,[23] was used.

The emissivities obtained were plotted against the shock tube data of Taylor[2] for nitrogen and for air. For all species, populations were read from the graphs provided by Taylor. To produce theoretical curves for a nitrogen gas, bremsstrahlung from electrons on N and N_2 was evaluated; for air, electron-oxygen bremsstrahlung was calculated in addition.

The calculations are displayed in Figs. 6–9. In Figs. 6 and 8 there were frequently a number of data at the same wavelength. The range of these data is indicated by a vertical line and the position of the median point is encircled. All of Taylor's data were taken at temperatures at which electron-nitrogen molecule collisions are the dominant mechanism for bremsstrahlung emission. Moreover, the calculation of emission from the molecule is sufficiently crude that its uncertainty is of the order of the atomic radiation. The contribution of recombination radiation to the volume emissivity has not been plotted in these figures. Calculation shows that it is a small effect except at the highest photon energies ($\lambda_\mu\simeq 2$), where the emissivity is increased roughly 10% by recombination radiation.

It can be seen that the emissivities are calculated to within 20–30% and no patent disagreement exists between theory and experiment.

Little more than consistency with the data can be claimed for the calculation of atomic bremsstrahlung. Yet, it is of interest to note that there is a strong wavelength dependence in the emissivity which agrees well with the shape of the calculated atomic bremsstrahlung curves. Clearly it would be desirable to have a more precise comparison between theory and experiment.[24,25]

Note added in proof In applying this theory to other atoms it has been found that it is sometimes not possible to solve the equations by iteration, and a noniterative method of solution has been devised. The failure of iterative techniques is connected with the existance of multiple solutions to the equations, and will be discussed in detail in a later paper.

---

[23] A. Engelhardt, A. Phelps, and C. Risk, Phys. Rev. **135**, A1566 (1964).

[24] R. Neynaber, L. Marino, E. Rothe, and S. Trujillo, Phys. Rev. **123**, 148 (1961).

[25] R. Neynaber, L. Marino, E. Rothe, and S. Trujillo, Phys. Rev. **129**, 2069 (1963).

ACKNOWLEDGMENTS

The authors would like to acknowledge a number of helpful conversations with Professor A. G. Petschek and Dr. W. R. Powell and the assistance of Dr. H. R. Lewis and Dr. R. M. Cantwell with numerical methods.

APPENDIX A: EVALUATION OF ϕ_1

In general Eq. (9) may be solved for ϕ_1 by standard Green's function techniques

$$\phi_1(k,y)_{m^l m^s}=\int dy'\mathcal{G}(y,y')H_1\phi_0(\mathbf{k}_0,y')_{m^l m^s}.$$

On the assumption that the functions $\phi_0(\mathbf{k}_0,y)_{m^l m^s}$ satisfy the Schrödinger equation defined by H_0, the Green's function is given by

$$\mathcal{G}(y,y')=A_j\sum_{L'}\sum_{S'}\sum_{l_1'}\sum_{M_L}\sum_{M_S}(-1)^{N+1-j}(N+1)^{1/2}\mathcal{G}_{L'S'l_1'}(r_j,r_j')G_{L'S'l_1'}{}^{M_L,M_S}(\mathcal{Y}_j)G^*{}_{L'S'l_1'}{}^{M_L,M_S}(\mathcal{Y}_j'). \tag{A1}$$

In the above, primes are used to distinguish the subscripts from those appearing in ϕ_0. The asymptotic form of $\mathcal{G}_{L'S'l_1'}(r_j,r_j')$ is

$$\lim_{r_j\to\infty}\mathcal{G}_{L'S'l_1'}(r_j,r_j')=-i^{2l_1'}\exp(-2i\delta_{l_1'}{}^{L'S'})\left(\frac{2mk}{\hbar^2}\right)\frac{2\pi^2}{2l_1'+1}\times\begin{cases}\tilde{R}_{l_1'}{}^{L'S'}(kr_j)R_{l_1'}{}^{L'S'}(kr_j')/r_jr_j' & \text{for} \quad r_j>r_j'\\ \tilde{R}_{l_1'}{}^{L'S'}(kr_j')R_{l_1'}{}^{L'S'}(kr_j)/r_jr_j' & \text{for} \quad r_j'>r_j\end{cases} \tag{A2}$$

where $\tilde{R}_{l'}{}^{L'S'}/r$ is the outgoing wave solution of the elastic-scattering radial equation (11), having the normalization

$$\lim_{r\to\infty}\frac{\tilde{R}_{l_1'}{}^{L'S'}(kr)}{r}=\frac{1}{\pi kr}\left(\frac{2l_1'+1}{2}\right)^{1/2}\exp(2i\delta_{l_1'}{}^{L'S'})e^{ikr}.$$

The complete r_j, r_j' dependence of $\mathcal{G}$ is more difficult to determine but is not needed here.

When the free electron is far from the atom, ϕ_{1i} takes on the limiting form

$$\phi_{1i}(k,y)_{m^l m^s}\to A_j\sum_{L'}\sum_{S'}\sum_{l_1'}\sum_{M_L}\sum_{M_S}\left(\frac{2m}{\hbar^2}\right)\frac{e^{ikr_j}}{r_j}\left[-\frac{i^{2l_1'}\sqrt{2}\pi}{(2l_1'+1)^{1/2}}\int dr_j'r_j'^2\frac{R_{l_1'}{}^{L'S'}(kr_j')}{r_j'}F_i(r_j')\right]G_{L'S'l_1'}{}^{M_L,M_S}(\mathcal{Y}_j) \tag{A3}$$

where

$$F_i(r_j')=-\left(\frac{ie\hbar}{mc}\right)\left(\frac{hc}{k_2\mathcal{V}}\right)^{1/2}\sum_L\sum_S\sum_{l_1}(l_1l_2L|0m^l)(\tfrac{1}{2}s_2S|m_1{}^s m^s)$$
$$\times\int d\mathcal{Y}_j'\int d\Omega_j'\sum_{\sigma_j'}G^*{}_{L'S'l_1'}{}^{M_L,M_S}(\mathcal{Y}_j')\hat{\epsilon}_i\cdot\nabla_j[R_{l_1}{}^{LS}(k_0r_j')/r_j']G_{LSl_1}{}^{m^l,m_1{}^s+m^s}(\mathcal{Y}_j').$$

Equation (3a) is used to express the functions G in explicit form. It is then possible to perform many of the summations and integrations and obtain comparatively simple explicit expressions for the limiting form of ϕ_{1i}. This process yields for the scattering amplitudes Eqs. (12) and (13) of the text.