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RM-3334-ARPA
OCTOBER 1962

BREMSSTRAHLUNG DURING THE COLLISION OF LOW-ENERGY ELECTRONS WITH NEUTRAL ATOMS AND MOLECULES

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The RAND Corporation
SANTA MONICA • CALIFORNIA

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PREFACE

The research reported in this Memorandum is part of a general study of the radiation emitted by charged particle beams.

The Memorandum discusses the impact radiation ("bremsstrahlung") emitted during the collision of low-energy electrons with neutral atoms and molecules. The study will be of general interest to persons studying the interaction of matter and radiation.

SUMMARY

This Memorandum discusses the bremsstrahlung radiation emitted during the collision of low-energy electrons with neutral atoms and molecules. The discussion is limited to the case of low-energies $E \leq 1$ ev, and soft photons, $\hbar\omega \ll E$, where E is the electron kinetic energy, and ω is the radiation frequency. The bremsstrahlung rate is expressed in terms of the elastic scattering amplitude, and use is made of various experimental and theoretical studies of the low-energy elastic scattering of electrons by neutral atoms and molecules. The rate of bremsstrahlung emission from a partially ionized gas due to electron-neutral collisions is calculated, and the results are presented in Eqs. (20) and (22). In Eq. (29) the electron-neutral bremsstrahlung rate is compared to the electron-ion bremsstrahlung rate.

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I. INTRODUCTION

The emission of bremsstrahlung radiation during the collision of electrons with neutral atoms and molecules is one of the oldest problems in quantum electrodynamics, and has been the subject of extensive research.[1] Theoretical studies of this process have almost invariably been based on the representation of the neutral target system by a screened coulomb field. This representation, which neglects any effect the incident electron may have on the electronic cloud of the atom or molecule, is adequate so long as the incident electron has an energy significantly greater than the energies of the bound electrons of the target system.

Recently, because of various applications in atmospheric and space physics, there has been interest in the bremsstrahlung associated with very low-energy electrons, having energies much less than the energies of the bound atomic or molecular electrons. For this region of energies the theoretical calculations based on a screened coulomb field are no longer adequate, since the incident electron strongly distorts the electronic cloud of the target atom or molecule. This distortion produces induced dipole, and higher-order multipole, fields surrounding the neutral target system. These induced fields alter the effective potential acting on the incident electron, and thereby change the character of the collision process. An understanding of the low-energy bremsstrahlung is further complicated by the scarcity of experimental information in this energy region.

The purpose of this Memorandum is to extend the theoretical discussion of bremsstrahlung into the very low-energy region, with

particular emphasis on electron energies below 1 ev. The present discussion will be limited to the soft-photon case, $\hbar\omega \ll E$, where E is the electron kinetic energy, and ω is the radiation frequency. For this case, the bremsstrahlung matrix element may be expressed directly in terms of the elastic scattering matrix element,[2] a relationship which is discussed in Section II. (For $\hbar\omega$ comparable to E, there is no direct relation between the bremsstrahlung and elastic scattering matrix elements. This greatly increases the difficulty of the problem, which is the reason for not considering that case here.) Use may then be made of the recent theoretical and experimental work on the low-energy elastic scattering of electrons by neutral atoms and molecules. (Reference 3 gives a partial review of this work.) In particular, for very low energies the rate of emission of bremsstrahlung radiation may be expressed in terms of a single parameter, the S-wave scattering length for the electron-atom or electron-molecule system. The scattering length is then obtained from theoretical or experimental determinations of the zero-energy scattering cross-section. This is discussed in Section III.

The scattering length approximation is correct for all neutral systems, atomic or molecular. For the case of spherically symmetric atoms, i.e., atoms with a ground state of zero angular momentum, it is possible to extend the bremsstrahlung calculation to higher energies by use of the modified effective-range theory developed by O'Malley, Rosenberg, and Spruch.[4,5] This theory, which takes into account the polarization effects, represents the scattering cross section as an expansion in powers of the incident electron momentum; the leading term of this expansion is the scattering length approximation. In

Section IV, this modified effective-range theory is employed to extend the bremsstrahlung calculation to the next higher order in the electron momentum. This extension introduces one new parameter, the atomic polarizability, which is readily available from experimental and theoretical studies.

The calculation in Section IV, though only rigorous for atoms of zero angular momentum, serves as an order of magnitude check on the region of validity, for all atomic and molecular systems, of the scattering length approximation. The results obtained there indicate that the scattering length approximation is adequate for energies below about 10^{-1} ev for all scattering systems with the possible exception of molecular nitrogen. The results also suggest that, for those atoms to which it applies, the calculation based on the modified effective range theory should be adequate up to energies of the order of 1 ev.

For the case of N_2, the region of validity of the scattering length approximation is uncertain due to experimental discrepancies in the determination of the scattering length. Since this is an important case for atmospheric problems, it is considered in more detail in Section V, where the bremsstrahlung rate obtained from the various experimental determinations of the scattering cross-section is calculated.

As an application of the results obtained in this Memorandum, in Section VI the rate of electron-neutral bremsstrahlung and the rate of electron-ion bremsstrahlung in a partially ionized gas are compared.

II. RELATION OF BREMSSTRAHLUNG TO SCATTERING

The differential cross section for bremsstrahlung is given by

$$d\sigma_B = \frac{2\pi V}{\hbar v} \left| M_B \right|^2 \rho_F \tag{1}$$

where V is the normalization volume, v is the incident velocity, M_B is the bremsstrahlung matrix element, and the density of final states, assuming non-relativistic electron energies and $\hbar\omega \ll E$, is given by

$$\rho_F = \frac{V^2 m^2 v \omega^2}{(2\pi)^6 \hbar^3 c^3} \, d\Omega_{p'} \, d\Omega_K \, d\omega \tag{2}$$

where $d\Omega_{p'}$ and $d\Omega_K$ are the differential solid angles for the recoil electron and photon, respectively, and m is the electron mass.

For non-relativistic electron energies, and for $\hbar\omega \ll E$, the bremsstrahlung matrix element can be expressed in terms of the scattering matrix element M_S as

$$M_B = \left(\frac{2\pi}{\hbar\omega V}\right)^{1/2} \frac{e}{m\omega} \vec{\epsilon} \cdot (\vec{P} - \vec{P}') \, M_S \tag{3}$$

where Gaussian units are used, $\vec{\epsilon}$ is the photon polarization, and $\vec{P}$ and $\vec{P}'$ are the incident and final electron momenta. (Equation 3 is essentially the non-relativistic limit of Eq. 16-3 in Ref. 2, differing only in the normalization and choice of units.) Using this, and expressing M_S in terms of the scattering amplitude $F(\theta)$ as [6]

$$M_S = -\frac{2\pi\hbar^2}{mV} F(\theta) \tag{4}$$

the expression for the bremstrahlung differential cross section is then

$$d\sigma_B = \frac{e^2 \, |F(\theta)|^2}{(2\pi)^2 \, m^2 \, \hbar\omega \, c^3} \, |\vec{\epsilon} \cdot (\vec{P} - \vec{P}')|^2 \, d\Omega_p, \, d\Omega_K \, d\omega \tag{5}$$

Summing this expression over the photon polarizations and integrating over the photon and recoil electron solid angles, the bremsstrahlung cross section, differential with respect to frequency, becomes

$$d\sigma_B = \frac{4}{3\pi}\left(\frac{e^2}{\hbar c}\right)\left(\frac{v}{c}\right)^2 \frac{d\omega}{\omega} \cdot \int |F(\theta)|^2 \, (1 - \cos\theta) \, d\Omega_p, \tag{6}$$

where $\hat{\vec{P}} \cdot \hat{\vec{P}}' = \cos\theta$.

For later work, it will be useful to express this result in terms of the scattering phase shifts. To do this, use is made of the relation [6]

$$F(\theta) = \frac{\hbar}{mv} \sum_{\ell=0}^{\infty} (2\ell + 1) \, e^{i\delta_\ell} \sin\delta_\ell \, P_\ell(\cos\theta) \tag{7}$$

where δ_ℓ is the phase shift for the ℓth partial wave. Keeping only S and P waves, the result is

$$\frac{d\sigma_B}{d\omega} = \frac{16\, e^2 \hbar}{3\, m^2\, \omega\, c^3} \Big[\sin^2 \delta_o + 3 \sin^2 \delta_1$$

$$- 2 \sin \delta_o \sin \delta_1 \cos(\delta_o - \delta_1) \Big] \qquad (8)$$

III. SCATTERING LENGTH APPROXIMATION

In the limit of very low energy, the differential scattering cross section becomes spherically symmetric, and the total scattering cross section approaches a constant value. (This is true for all atomic and molecular systems which do not possess a permanent electric dipole moment.) In this limit the scattering amplitude becomes $F(0) = A$, where A is the S-wave scattering length, which is related to the zero-energy total scattering cross section σ_o by $\sigma_o = 4\pi A^2$. Using this expression for the scattering amplitude, the bremsstrahlung cross section, Eq. (6), becomes

$$d\sigma_B = \frac{16 A^2}{3} \left(\frac{e^2}{\hbar c}\right)\left(\frac{v}{c}\right)^2 \frac{d\omega}{\omega} \tag{9}$$

The region of validity of this scattering length approximation to the bremsstrahlung cross-section will be determined in Section IV, where the next higher-order term in the low-energy expansion of the scattering amplitude is taken into account. (Equation (9) will be found to be valid for most gases for electron energies below about 0.1 ev.)

In recent years there has been a great deal of theoretical and experimental work on the low-energy scattering of electrons by neutral atoms and molecules. As a result of this work, values of the S-wave scattering length have been determined for a large number of atoms and molecules. In Table 1 these values are tabulated for various gases. (As defined here, A is the effective scattering length averaged over the different possible spin states of the electron-atom or electron-molecule system. For example, for electron-hydrogen scattering,

Table 1

VALUES OF SCATTERING LENGTH

Material	Scattering Length (in units of a_o)*	Reference No.**
H	+3.35	7
H_2	+1.9	8
	+1.49	9
N	+1.857	10
	+1.3	11
N_2	$0 < A \lesssim +0.7$	8
	$0 < A \lesssim +0.5$	9
	-2.7	12
O	+0.75	13
He	+1.23	9
	+1.18	14
Ne	+0.32	14
A	~ -1.7	9
	-1.46	15
	-1.9	14
Kr	-2.1	8
	-3.7	14
Xe	-3.8	8
	-6.2	14

$$^{*}a_o = \frac{\hbar^2}{me^2} = 0.529 \times 10^{-8} \text{ cm}$$

** See References, p. 21

$A = \frac{1}{2}\left(3 A_T^2 + A_S^2\right)^{1/2}$, where A_T and A_S are the scattering lengths for the triplet and singlet states.) Although numerical discrepancies do exist, Table 1 shows that the order of magnitude of the scattering length is well established for the various gases, with the possible exceptions of N_2, for which sizable discrepancies exist, and O_2, for which there are no data.

The rate of bremsstrahlung radiation from a partially ionized gas due to electron-neutral collisions will now be calculated, using Eq. (9) for the bremsstrahlung cross section. For the case of mono-energetic electrons, assuming that the electron velocity is large compared to the atomic or molecular velocity, the rate of bremsstrahlung radiation per unit volume of the gas is given by

$$\frac{dP_B}{d\omega} = v\, n_a\, n_e\, \hbar\omega\, \frac{d\sigma_B}{d\omega} \tag{10}$$

where n_e is the electron density, and n_a is the atomic or molecular density. This becomes

$$\frac{dP_B}{d\omega} = \frac{16}{3}\, e^2\, A^2\, n_a\, n_e \left(\frac{2E}{mc^2}\right)^{3/2} \tag{11}$$

where E is the electron kinetic energy. For E in ev, and n_a and n_e in particles/cm^3, this becomes

$$\frac{dP_B}{d\omega} = 2.68 \times 10^{-43}\, E^{3/2}\, n_a\, n_e \left(\frac{A}{a_o}\right)^2 \tag{12}$$

ergs/cm^3 · sec per rad/sec

where $a_o = \frac{\hbar^2}{me^2} = 0.529 \times 10^{-8}$ cm is the Bohr radius. (Note that, for order of magnitude estimates, $A/a_o \sim 1$.)

For a Maxwellian distribution of electrons, the bremsstrahlung rate is given by

$$\frac{dP_B}{d\omega} = n_a \, n_e \, \hbar\omega \int_o^\infty \frac{d\sigma_B}{d\omega} \, v\rho(v) \, dv \tag{13}$$

where

$$\rho(v) \, dv = 4\pi \left(\frac{m}{2\pi KT}\right)^{3/2} e^{-\frac{mv^2}{2KT}} \, v^2 \, dv \tag{14}$$

where T is the electron temperature. Using Eq. (9) this gives

$$\frac{dP_B}{d\omega} = \frac{64}{3\pi^{1/2}} \, e^2 \, A^2 \, n_a \, n_e \left(\frac{2KT}{mc^2}\right)^{3/2} \tag{15}$$

For KT in ev, and n_a and n_e in particles/cm^3, this becomes

$$\frac{dP_B}{d\omega} = 6.04 \times 10^{-43} \, (KT)^{3/2} \, n_a \, n_e \left(\frac{A}{a_o}\right)^2 \tag{16}$$

ergs/cm^3 · sec per rad/sec

IV. MODIFIED EFFECTIVE-RANGE APPROXIMATION

The scattering length approximation used in Section III is the first term in the low-energy expansion of the scattering amplitude. The form of the higher-order terms in this expansion, the effective-range theory, is well known for the case of short-range potentials.[16] Recently, a modified effective-range theory has been developed by O'Malley, Rosenberg, and Spruch,[4,5] which takes into account the long-range polarization effects present in electron-neutral scattering. In this section the results of O'Malley, et al., will be used to extend the calculation of Section III to the next higher order in the electron momentum.

The modified effective-range theory applies to the elastic scattering of charged particles by spherically symmetric scattering systems that do not possess any permanent multipole moments. It therefore does not apply to molecules which, in general, are not spherically symmetric, and for which inelastic channels involving excited rotational levels of the electronic ground state are very important even at the low energies considered here. It also does not apply to atomic oxygen which has a permanent electric quadrupole moment. Even for those systems to which it does not rigorously apply, however, it is expected that a calculation based on the modified effective-range theory will provide an order of magnitude indication of the region of validity of the scattering length approximation to the bremsstrahlung cross section.

The zero and first-order terms in the low-energy expansion of the bremsstrahlung cross section in powers of the electron momentum involve

only the S-wave and P-wave scattering phase shifts. (This can be determined from the expressions for the higher partial wave phase shifts given in Ref. 5.) Using the modified effective-range theory and keeping terms to first order, these phase shifts become[4,5]

$$\frac{mv}{\hbar} \cot \delta_o = - \frac{1}{A} + \frac{\pi \alpha mv}{3A^2 a_o \hbar} \tag{17}$$

and

$$\tan \delta_1 = \frac{\pi \alpha m^2 v^2}{15 a_o \hbar^2} \tag{18}$$

where α is the low-frequency electric polarizability of the atom. In Table 2, values of α are given for various atoms and molecules. (The polarizabilities of H_2, N_2 O_2, He and A were obtained from the measured values of the dielectric constant ϵ by use of the relation $\epsilon - 1 = 4\pi N\alpha$, where N is the density.)

Using Eqs. (8), (17) and (18) and keeping terms to first order in the electron momentum, the bremsstrahlung cross section becomes

$$d\sigma_B = \frac{16A^2}{3} \left(\frac{e^2}{\hbar c}\right)\left(\frac{v}{c}\right)^2 \frac{d\omega}{\omega} \left(1 + \frac{8\pi \alpha mv}{15a_o A \hbar}\right) \tag{19}$$

By comparing Eqs. (9) and (19), it can be seen that the scattering length approximation as given in Eq. (9) will be valid for $\alpha mv/a_o A\hbar \ll 1$, or $(\alpha/a_o^2 A) \cdot \left(\frac{v}{c}\right) \ll \frac{1}{137}$. For helium this

Table 2

VALUES OF POLARIZABILITY

Material	Polarizability (in units of a_o^3)*	Reference No.
H	4.50	17
H_2	5.43	18
N	7.084	10
N_2	11.7	18
O	5.589 5.499	10 19
O_2	10.6	18
He	1.39	18
A	11.1	18

$^*a_o^3 = \left(\frac{\hbar^2}{me^2}\right)^3 = 0.148 \times 10^{-24}\ cm^3$

corresponds to $E \ll 10$ ev, and for atomic nitrogen, $E \ll 0.25$ ev. For the other atomic gases the upper limit of the region of validity of the scattering length approximation lies between these two extreme cases.

As discussed earlier, Eq. (19) does not rigorously apply to molecules. However, it is expected that the low-energy expansion of the cross section for the molecular case should be of the same general form. Accordingly Eq. (19) can be used as an estimate of the order of magnitude of the leading correction term to the scattering length approximation in the molecular case. Doing this, for H_2 the scattering length approximation is found to have the region of validity $E \ll 1$ ev, and for N_2 either $E \ll 1$ ev or $E \ll 0.03$ ev, depending upon which value of A is used.

In order to determine the region of energies for which Eq. (19) adequately represents the bremsstrahlung cross section (for those systems to which it applies), it would be necessary to calculate the next higher-order term in the modified effective-range expansion of the scattering amplitude, a problem beyond the scope of this Memorandum. However, from the results of O'Malley, et al.,[5] Eq. (19) is valid up to about 0.5 ev for hydrogen. For other atoms the region of validity is expected to be similar, so that in general Eq. (19) will be valid for spherically symmetric atoms for energies below about 1 ev.

As in Section III, the rate of bremsstrahlung radiation from a partially ionized gas due to electron-neutral collisions is next calculated, using Eq. (19) for the bremsstrahlung cross section. For

the case of monoenergetic electrons, the result is

$$\frac{dP_B}{d\omega} = \frac{16}{3} \; e^2 \; A^2 \; n_a \; n_e \left(\frac{2E}{mc^2}\right)^{3/2} \left[1 + \frac{8\pi}{15}\left(\frac{\hbar c}{e^2}\right)\left(\frac{\alpha}{a_o^{\,2} \; A}\right)\left(\frac{2E}{mc^2}\right)^{1/2} \right] \tag{20}$$

which, for E in ev, and n_a and n_e in particles/cm^3, becomes

$$\frac{dP_B}{d\omega} = 2.68 \times 10^{-43} \; E^{3/2} \; n_a \; n_e \left(\frac{A}{a_o}\right)^2 \cdot \left[1 + 0.459\left(\frac{\alpha}{a_o^{\,2} \; A}\right) E^{1/2} \right] \tag{21}$$

ergs/cm^3 · sec per rad/sec

For the case of a Maxwellian distribution of electrons, the result is

$$\frac{dP_B}{d\omega} = \frac{64}{3\pi^{1/2}} \; e^2 \; A^2 \; n_a \; n_e \left(\frac{2KT}{mc^2}\right)^{3/2} \cdot \left[1 + \frac{\pi^{3/2}}{2}\left(\frac{\hbar c}{e^2}\right)\left(\frac{\alpha}{a_o^{\,2} \; A}\right)\left(\frac{2KT}{mc^2}\right)^{1/2} \right] \tag{22}$$

which for KT in ev, and n_a and n_e in particles/cm^3, becomes

$$\frac{dP_B}{d\omega} = 6.04 \times 10^{-43} \; (KT)^{3/2} \; n_a \; n_e \left(\frac{A}{a_o}\right)^2 \cdot \left[1 + 0.763\left(\frac{\alpha}{a_o^{\,2} \; A}\right)(KT)^{1/2} \right] \tag{23}$$

ergs/cm^3 · sec per rad/sec

V. USE OF EXPERIMENTAL RESULTS FOR MOLECULAR NITROGEN

For N_2 the results previously obtained have not been very satisfactory due to discrepancies in the various experimental determinations of the scattering cross section. Because of the importance of this case for atmospheric problems, in this section is discussed the bremsstrahlung rate obtained from the two most recent, and most divergent, experimental measurements of the low-energy electron-N_2 scattering cross section. This discussion will give a more detailed estimate of the electron-N_2 bremsstrahlung rate than the discussion in the previous sections, and will illustrate the uncertainty in the experimental situation.

The experiments in question, based either on measurements of the electron drift velocity in applied electric fields,[9] or on microwave measurements of electron mobility,[12] determined the momentum transfer cross section σ_d, defined as

$$\sigma_d = \int |F(\theta)|^2 (1 - \cos\theta)\, d\Omega \tag{24}$$

In terms of σ_d, the bremsstrahlung cross section, as given in Eq. (6), becomes

$$d\sigma_B \doteq \frac{4}{3\pi}\left(\frac{e^2}{\hbar c}\right)\left(\frac{v}{c}\right)^2 \sigma_d \frac{d\omega}{\omega} \tag{25}$$

For the case of monoenergetic electrons the rate of bremsstrahlung radiation from a partially ionized gas due to electron-neutral collisions then becomes

$$\frac{dP_B}{d\omega} = \frac{4}{3\pi} \; e^2 \, \sigma_d \, n_a \, n_e \left(\frac{2E}{mc^2}\right)^{3/2} \tag{26}$$

For E in ev, and n_a and n_e in particles/cm^3, this becomes

$$\frac{dP_B}{d\omega} = 8.42 \times 10^{-43} \, E^{3/2} \, n_a \, n_e \left(\frac{\sigma_d}{\pi a_o^{\,2}}\right) \tag{27}$$

ergs/cm^3 . sec per rad/sec

where the values of $\sigma_d/\pi a_o^{\,2}$ for N_2 obtained from Refs. 9 and 12 are plotted in Fig. 1. From the figure, it can be noted that at very low energies there is a factor of 10 uncertainty in the bremsstrahlung rate from N_2.

As discussed in Section IV, if the experimental results of Pack and Phelps [9] are correct, the scattering length approximation for N_2 begins to fail for $E \sim 10^{-2}$ ev. However, if the experimental results of Anderson and Goldstein [12] are correct, the scattering length approximation is valid up to at least $E \sim 10^{-1}$ ev.

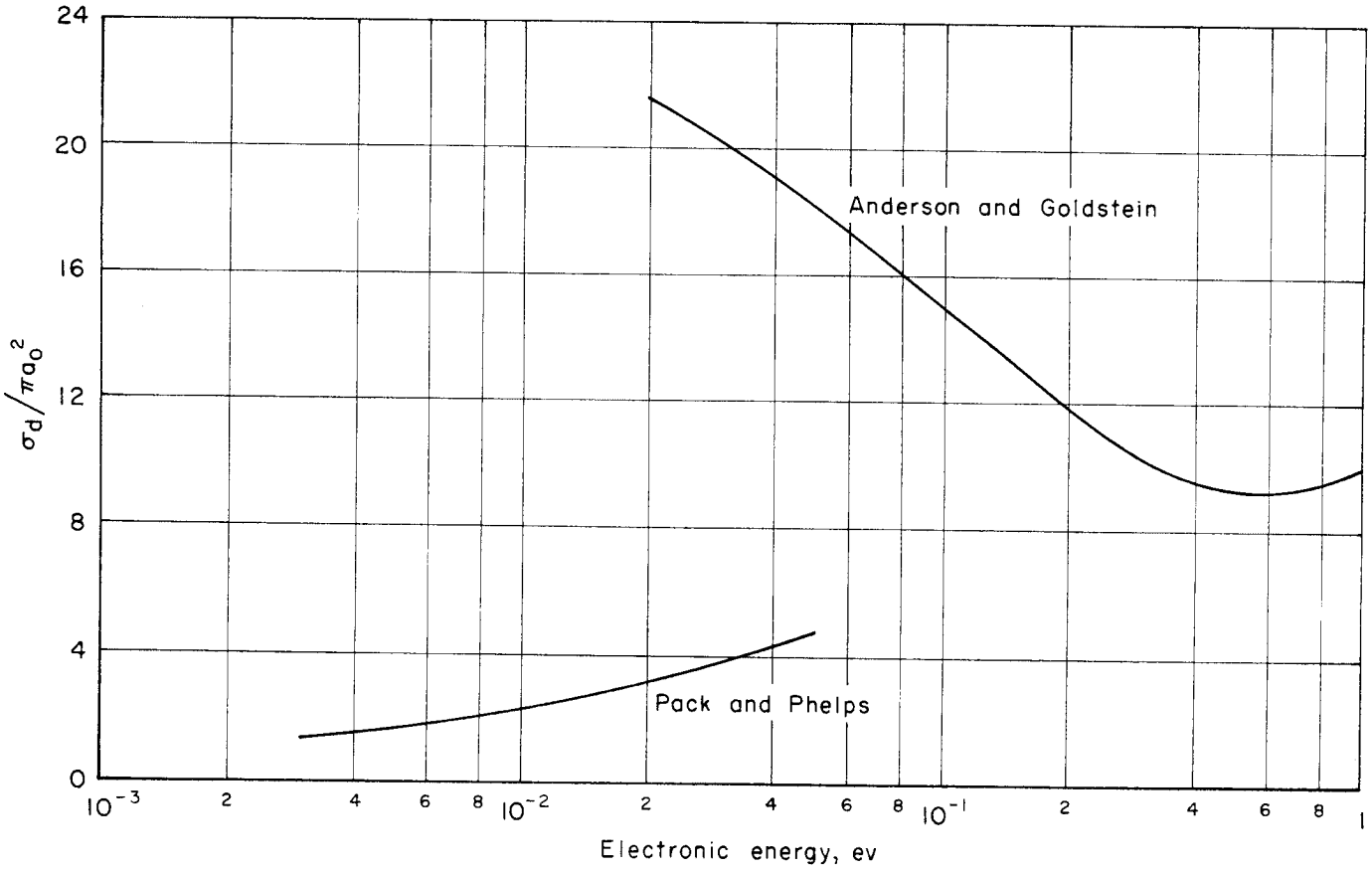

Fig. 1 — Momentum transfer cross section for N_2

VI. COMPARISON OF ELECTRON-NEUTRAL AND ELECTRON-ION BREMSSTRAHLUNG

In a partially ionized gas, electron-neutral bremsstrahlung and electron-ion bremsstrahlung are competing processes. It is interesting to determine which is the dominating bremsstrahlung process for various degrees of ionization. In the soft-photon limit, $\hbar\omega \ll KT$, and for the case of low-electron energies, $KT < 700$ ev, the rate of bremsstrahlung radiation due to electron-ion collisions is given by[20]

$$\frac{dP_{ion}}{d\omega} = \frac{16}{3} e^2 r_e^2 n_e n_i Z^2 \left(\frac{2mc^2}{\pi KT}\right)^{1/2} \ln\left[1.33 \frac{KT}{\hbar\omega}\left(\frac{KT}{E_o}\right)^{1/2}\right] \qquad (28)$$

where $r_e = e^2/mc^2 = 2.82 \times 10^{-13}$ cm, $E_o = me^4/\hbar^2 = 27.21$ ev, n_i is the ion density, Z is the ionic charge, and a Maxwellian distribution of electrons has been assumed.

If the scattering length approximation, as given in Eq. (15), is used for the rate of electron-neutral bremsstrahlung, then the ratio of the electron-ion bremsstrahlung rate to the electron-neutral bremsstrahlung rate, $R = (dP_{ion}/d\omega)/(dP_B/d\omega)$, becomes

$$R = \frac{1}{8}\left(\frac{e^2}{\hbar c}\right)^4 \frac{n_i Z^2}{n_a}\left(\frac{a_o}{A}\right)^2\left(\frac{mc^2}{KT}\right)^2 \ln\left[1.33 \frac{KT}{\hbar\omega}\left(\frac{KT}{E_o}\right)^{1/2}\right] \qquad (29)$$

In Fig. 2 the quantity $R(n_a/Z^2 n_i)(A/a_o)^2$ is plotted for various values of KT and $\hbar\omega/KT$. From these results the relative importance of electron-ion and electron-neutral bremsstrahlung can be determined for a wide range of physical conditions.

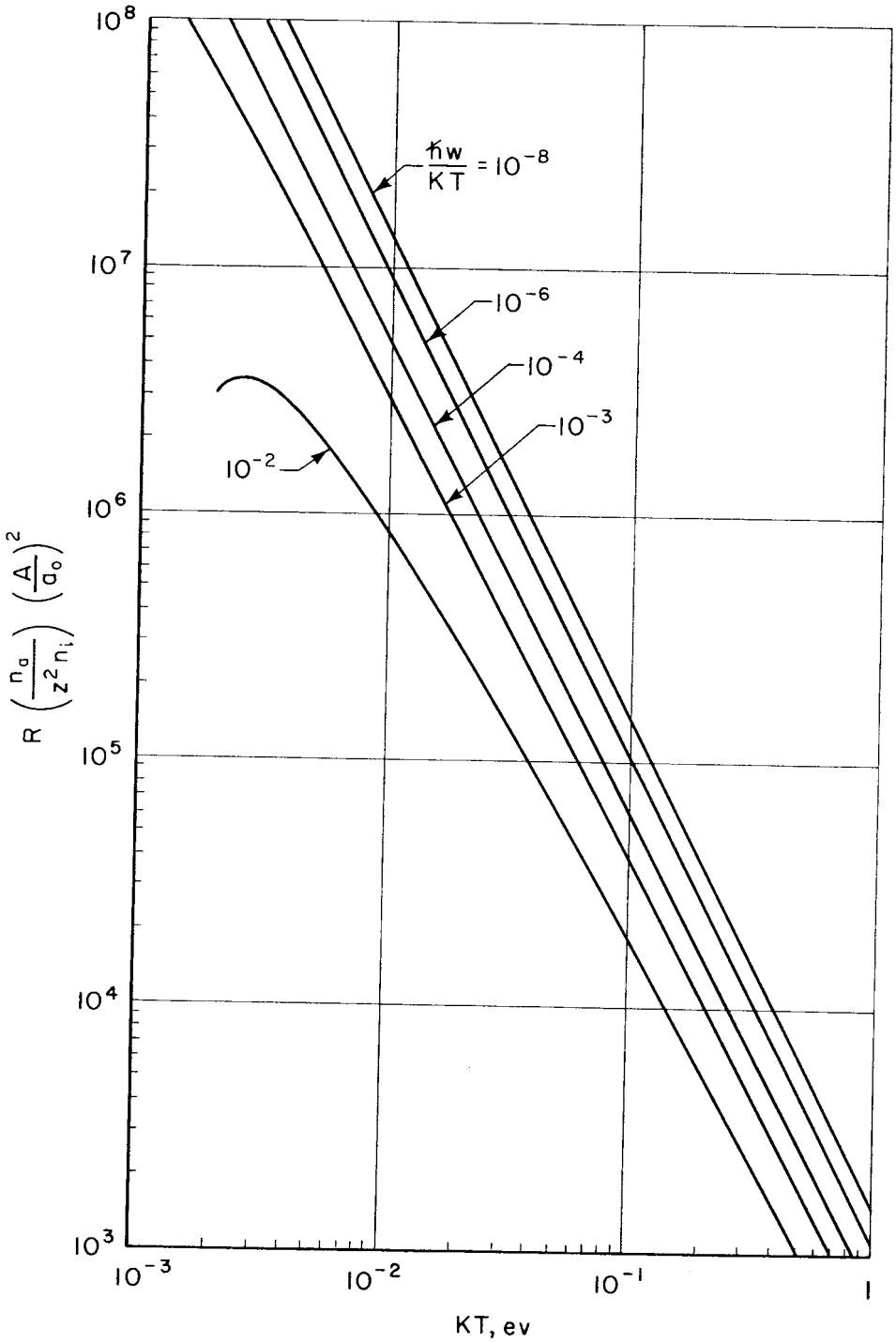

Fig. 2 — Comparison of electron-ion and electron-neutral bremsstrahlung rates

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