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Radiation by an electron in a Coulomb field

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Abstract. The cross section for free-free transitions—bremsstrahlung at non-relativistic velocities—can be reduced to simple formulae in various limiting cases. In two of these cases, the quantum-mechanical result is known to agree with Kramers' classical calculations (namely g = 1 and $g = (\sqrt{3}/\pi) \ln(...)$ in the usual 'Gaunt factor' notation of astrophysicists). The intermediate case does not seem to have been completely cleared up, and it is investigated here. The result found does not agree with the formula of Elwert; it depends on a function of a single variable, and coincides with the classical result. This bridges the gap between the two low-frequency formulae. A short table of the function is given.

A method is given for calculating the cross section in the more general conditions in which g is nearly equal to 1 (hv not small compared with $\frac{1}{2}mv_1^2$). There is a region of overlap between the result so obtained and the preceding one, which provides a check on the correctness of both.

1. Introduction

The problem of the emission of radiation by an electron passing a nucleus is such an old one that it might be thought it was completely solved, anyhow in the non-relativistic case. The general formulae for free-free transitions, containing hypergeometric functions, can be reduced to simpler functions in some six or seven limiting cases. One such case, referring to the low-frequency end of the spectrum which is of some astrophysical interest, does not appear to have been cleared up hitherto.

Kramers (1923), before the discovery of quantum mechanics, calculated the radiation emitted on the basis of classical theory. He gave a general formula (equation (12) below) and two simpler formulae in two limiting cases which were widely used by astrophysicists. Quantum-mechanical calculations have shown that his two simpler formulae are valid under suitable conditions; but the question of his more general case remains open, and indeed such work as has been done indicates a different result (Elwert 1939, 1948). It will be shown here that the cross section is given correctly by Kramers' general formula, depending on a function of a single variable, in the case when $hv \ll \frac{1}{2}mv_1^2 \ll I$, the ionization potential. These conditions mean that the electron loses a small fraction of its energy, and that the principal quantum numbers are large. They look plausible as necessary conditions for formulae based on a classical hyperbolic orbit: it turns out that they are also sufficient.

In § 4 we obtain a more general (quantum) formula for the case when the electron loses a finite fraction of its energy. In § 5 we give a brief alternative derivation of one or two of the other known approximate results.

2. Notation

The energies of the incoming and outgoing electron may be conveniently specified as I/ξ^2 and I/η^2 , where -I is the energy of the lowest bound state (K shell);

$$\xi = (\mu_0 c^2 / 4\pi) Z e^2 / \hbar v_1;$$

i ξ and i η are the analogues of the principal quantum number n.

According to quantum mechanics, the cross section for an electron with initial energy E_1 to emit a photon $\hbar\omega$ in the range of frequency $d\omega/2\pi$ is

$$\frac{16\pi^2}{3} \frac{a_0^2}{137^3} \frac{I}{E_1} \frac{\xi\eta}{(e^{2\pi\xi} - 1)(1 - e^{-2\pi\eta})} |D(i\xi, i\eta)| \frac{d\omega}{\omega}$$
(1)

where

$$D(i\xi, i\eta) = (\eta - \xi)^{-1} [F(-i\xi + 1, -i\eta, 1; z)^2 - F(-i\xi, -i\eta + 1, 1; z)^2]$$
(2)

and $z = -4\xi\eta/(\eta-\xi)^2$.

The derivation of (1) is too long to give here: it will be sufficient to point out that it can easily be transformed into the formula derived by Sommerfeld (Sommerfeld and Maue 1935, Sommerfeld 1940). The only step in the process that might present difficulty is dealt with in appendix 1. The form (2) was first given by McLean (1934).

3. The case of ξ , η large, $\eta - \xi$ not large

When ξ and η are nearly equal, these hypergeometric functions in (2) are to be regarded as analytic continuations of the series into the left half-plane, as the series themselves are divergent. It is advantageous to transform them into hypergeometric functions of the new variable

$$\frac{1}{1-z} = \left(\frac{\eta-\xi}{\eta+\xi}\right)^2 \tag{3}$$

by means of the formula

$$F(a, b, c; z) = (1-z)^{-a} \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)} F\left(a, c-b, a-b+1; \frac{1}{1-z}\right) + (1-z)^{-b} \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)} F\left(b, c-a, b-a+1; \frac{1}{1-z}\right).$$
(4)

The new series are always convergent, and the new variable (3) is small in the low-frequency limit.

Expressing the two quantum numbers in terms of their mean and their difference,

$$X = \frac{1}{2}(\eta + \xi) \qquad \xi = X - \frac{1}{2}q$$

$$q = \eta - \xi \qquad \eta = X + \frac{1}{2}q$$
(5)

the first of the two functions on the right in (2) becomes

$$\left(\frac{q^{2}}{4X^{2}}\right)^{1-iX+\frac{1}{2}iq} \frac{\Gamma(-1-iq)}{\Gamma(-iX-\frac{1}{2}iq)\Gamma(iX-\frac{1}{2}iq)} F(-iX+\frac{1}{2}iq+1, iX+\frac{1}{2}iq+1, iq+2; q^{2}/4X^{2}) + \left(\frac{q^{2}}{4X^{2}}\right)^{-iX-\frac{1}{2}iq} \frac{\Gamma(1+iq)}{\Gamma(1-iX+\frac{1}{2}iq)\Gamma(1+iX+\frac{1}{2}iq)} \times F(-iX-\frac{1}{2}iq, iX-\frac{1}{2}iq, -iq; q^{2}/4X^{2}).$$
(6)

The next step is to evaluate the two series in this somewhat complicated expression and the factors outside them, for large X.

For $X \to \infty$ with q fixed, the series can be simplified. All the four series required are of the form

$${}_{2}F_{1}(-iX + \frac{1}{2}m, iX + \frac{1}{2}m, m; q^{2}/4X^{2})$$
(7)

with different values of *m*. As the convergence is uniform in X (appendix 2), it is permissible to take the limit of each term. The term containing the sth power of the variable $q^2/4X^2$ is

$$\frac{(\frac{1}{2}q)^{2s}}{m(m+1)\dots(m+s-1)s!}\left[1+O\left(\frac{1}{X^2}\right)\right].$$

The hypergeometric series (7) thus reduces to the series ${}_{0}F_{1}(m; \frac{1}{4}q^{2})$ in the notation of Barnes (Watson 1922, p 100), which is simply the Bessel function

 $\Gamma(m)(\frac{1}{2}q)^{-(m-1)}I_{m-1}(q).$

The factors attached to the series in (6) can also be simplified, using the relation

$$\ln[\Gamma(iX+w)\Gamma(-iX+w)] = (2w-1)\ln X - \pi X + \ln(2\pi) + O(1/X^2)$$

which follows from Stirling's formula (with remainder). The first hypergeometric function in (2) then becomes

$$\frac{e^{\pi X}}{2i\sinh \pi q} \left(\frac{q}{2X}\right)^{1-2iX} (I_{iq+1}(q) - I_{-iq-1}(q)).$$
(8)

The second function in (2) can be dealt with by merely changing the sign of q in the preceding calculation, provided that care is taken over two details: in the complex powers of q^2 which arise from the powers of (1-z) in (4), $\arg q^2$ is still to be taken as zero and not $\pm 2\pi$; and in expressing ${}_0F_2$ in terms of a Bessel function, it is natural to use $I_{\nu}(q)$ rather than $I_{\nu}(-q)$. The result is the same as (8) with the sign of q changed only in the orders of the Bessel functions.

Expressing the Bessel functions in terms of the usual

$$K_{v}(x) = \frac{1}{2}\pi (I_{-v}(x) - I_{v}(x))/\sin v\pi$$

and remembering that

$$K_{-\nu}(x) = K_{\nu}(x),$$
 (9)

the expression (2) becomes

$$D(\mathrm{i}\xi,\mathrm{i}\eta) = \frac{\mathrm{e}^{2\pi X}}{q\pi^2} \left(\frac{q}{2X}\right)^{2-4\mathrm{i}X} (K_{\mathrm{i}q+1}(q)^2 - K_{\mathrm{i}q-1}(q)^2)$$

and so, after using the recurrence relations, we have

$$|D| = \frac{e^{2\pi X}}{\pi^2 X^2} (-q K_{iq}(q) K'_{iq}(q)).$$

The factor in parentheses is real and positive; it is evident from (9) that it is real. On inserting this value in (1), we find the cross section

$$\frac{16\pi}{3\sqrt{3}}\frac{a_0^2}{137^3}\frac{I}{E_1}\frac{\mathrm{d}\omega}{\omega}g(q) \tag{10}$$

where g, the 'Gaunt factor', is the function

$$g(q) = -(\sqrt{3/\pi}) e^{\pi q} q K_{iq}(q) K'_{iq}(q); \qquad (11)$$

this is valid for $\xi \to \infty$ with $q = \eta - \xi$ finite, with an error of the order of $1/\xi^2$. This result is identical, apart from notation, with Kramers' general classical result

$$g(q) = (\frac{1}{4}\pi\sqrt{3})iq H_{iq}^{(1)}(iq) H_{iq}^{(1)'}(iq).$$
(12)

For large q or small q, it goes over into the more commonly quoted formulae

$$g \simeq \begin{cases} 1 & (q \gg 1) \\ \pi^{-1} \sqrt{3[\ln(2/q) - \gamma]} & (q \ll 1). \end{cases}$$
(13)

In the second formula, $\gamma = 0.577...$; the error is of the order of $q^2(-\ln q)^3$. The first formula is the leading term of an expansion (Watson 1922, §8.42, Abramowitz and Stegun 1964, p. 368),

$$g = 1 + 0.2177 q^{-2/3} - 0.0131 q^{-4/3} \dots$$

Some numerical values of the function (11) are given in table 1.

q	g(q)	q	g(q)	q	g(q)	q	g(q)	q	g(q)
0.001	3.8844	0.1	1.7096	0.6	1.2741	1.2	1.1804	3	1.1012
0.003	3.2968	0.2	1.5046	0.7	1.2502	1.4	1.1639	4	1.0841
0.01	2.6809	0.3	1.4065	0.8	1.2310	1.6	1.1508	6	1.0646
0.02	2.3512	0.4	1.3464	0.9	1.2151	1.8	1.1401	8	1.0535
0.05	1.9603	0.5	1.3049	1.0	1.2018	2.0	1.1310	10	1.0463

 Table 1. Kramers' function (11)

The result (11) is not in agreement with the formulae found by Elwert (1948), except in the limit, in which case neither offers anything new.

4. The case of ξ , η and $\eta - \xi$ all large

It appears from the last section that

$$g = 1 + 0.2177(\eta - \xi)^{-2/3} - 0.0131(\eta - \xi)^{-4/3} \dots$$
(14)

when $\xi, \eta \to \infty$ with $\eta - \xi$ fixed, and $\eta - \xi$ is subsequently taken to be a fairly large number, say 5 or 10. (This means $E_1/I \to 0$, and $(E_1 - E_2)\sqrt{(I/E_1^3)}$ a rather small 'large number'.)

This is unsatisfactory; to see better where and how (14) begins to break down, it needs to be supplemented by an investigation in which $E_1 - E_2$ is not so restricted.

We therefore consider the case $\xi, \eta \to \infty$ with the ratio ξ/η fixed and not equal to 1, which means $E_1 - E_2$ is a fixed fraction of E_1 . But the result will be applicable even if $(E_1 - E_2)/I$ goes to zero faster than E_1/I provided it is large compared with $(E_1/I)^{3/2}$. It can be found without much labour if the method is suitably chosen.

It is not difficult to verify the usual result that the contour integral

$$\int u^{a-c}(u-1)^{c-b-1}(u-x)^{-a}\,\mathrm{d} u$$

satisfies the differential equation for F(a, b, c; x) if taken along a suitable path (Whittaker and Watson 1927, p 293). For the hypergeometric function $F(-i\xi+1, -i\eta, 1; x)$, with x < 0, this suggests considering

$$(1/2\pi i)\int u^{-i\eta-1}(u-x)^{i\eta}(1-u)^{i\xi-1}\,\mathrm{d}u$$

taken along a loop going round a cut from x to 0, in the positive sense, but not crossing another cut from 1 to ∞ . Choosing the arguments to be all zero where the path crosses the real axis in 0 < u < 1, it can be seen that this is not only a solution but is the right solution of the differential equation, because it becomes 1 in the limit $x \to 0$. The quantity required is the value of this integral when $x = -4\xi\eta/(\eta-\xi)^2$, in particular when ξ and η are large and the ratio $\rho = \xi/\eta$ is fixed ($0 < \rho < 1$).

In order to arrange the two cuts symmetrically in the complex plane, we introduce the new variable

$$t = \frac{2 - (1 - \rho)u}{2\rho + (1 - \rho)u}.$$

The path now runs in the negative sense round a cut from -1 to +1, and there are cuts from $1/\rho$ to ∞ and $-\infty$ to $-1/\rho$; changing the sign and traversing the path in the positive sense, we have

$$\frac{1}{2\pi i} \frac{(1+\rho)^{i\xi+i\eta}}{(1-\rho)^{i\xi+i\eta-1}} \int \left(\frac{1+\rho t}{1-\rho t}\right)^{i\eta} \left(\frac{t-1}{t+1}\right)^{i\xi} \frac{dt}{(1-\rho t)(t-1)}$$
(15)

for the value of the first of the functions in (2). The second one can be obtained by changing the $i\xi$ and $i\eta$ in the exponents by one unit, which has the effect of replacing the last denominator in (15) by $(1 + \rho t)(t + 1)$.

To apply the saddle-point method, one regards the integrand in (15) as

$$f(t)\exp(\eta g(t)) \tag{16}$$

with ρ fixed and $\eta \rightarrow \infty$, where

$$g(t) = i \left(\ln \frac{1+\rho t}{1-\rho t} + \rho \ln \frac{t-1}{t+1} \right).$$

It turns out that there are two saddle points: both are at t = 0 but they are on different sheets of the Riemann surface, ie approaching t = 0 from above and from below the cut (figure 1). There is a path of steepest descent, Im g(t) = 0, passing through both, and

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Figure 1. Path in the t plane.

making angles of $\pi/6$ with the real axis. Near the saddle point on the lower side of the cut, where $\arg(t-1)$ approaches $-\pi$,

$$g(t) = \pi \rho - 2i\rho \left[\frac{1}{3}(1-\rho^2)t^3 + \frac{1}{5}(1-\rho^4)t^5 + \ldots\right].$$

The value of Re g(t) decreases all the way to a value $-\pi\rho$ at the other saddle point, which is therefore unimportant. The important part of the contour is the piece near 0 where |t| is of the order of $\eta^{-1/3}$.

There are several ways of carrying out this sort of calculation in detail. The method given in appendix 3 is a good deal shorter in practice than the traditional methods, and there is less risk of a slip in the calculation. The result (A.5) is equivalent to a Gaunt factor

$$g = 1 - \frac{A}{2^{2/3} 5A'} \frac{E_1 + E_2}{I^{1/3} (E_1 - E_2)^{2/3}} + \frac{A'}{2^{1/3} 35A} \frac{3E_1^2 - 4E_1 E_2 + 3E_2^2}{I^{2/3} (E_1 - E_2)^{4/3}} \dots$$
(17)

The second term is positive and the third negative; the coefficients are 0.1728 and -0.0165.

This formula shows the limit of validity of Kramers' simplest formula (g = 1). The range of validity overlaps with that of (14). In fact, if we suppose that $(E_1 - E_2)/E_1$ tends to zero but not as fast as $(E_1/I)^{1/2}$ $(\eta - \xi \rightarrow \infty$ not as fast as ξ), we obtain exactly the first three terms in (14). This gives a check on the correctness of both calculations.

5. The case of $\eta - \xi$ small, $\xi \eta$ finite

It is worth noticing that our transformation (4) or (6) leads easily to some of the existing approximate formulae. We again denote the mean and the difference of the quantum numbers by X and q according to (5). The two hypergeometric functions in (6) are now $1 + O(q^2)$ and $1 + \frac{1}{4}iq + O(q^3)$. Quantities like $\Gamma(1 + iX + \frac{1}{2}iq)$ can be evaluated with two terms of a Taylor series in q, and the two parts of the first F in (2) then become

$$\left(\frac{q^2}{4X^2}\right)^{-iX}\frac{\sinh \pi X}{\pi X}[(-\frac{1}{4}iq) + (1 + \frac{1}{4}iq + iq\psi(1) - iq \operatorname{Re}\psi(1 + iX)]]$$

After squaring and subtracting the other term, it is found that the Gaunt factor is

$$g = (\sqrt{3/\pi}) [-\ln(q/2X) + \psi(1) - \operatorname{Re} \psi(1 + iX)] e^{\pi q}.$$
 (18)

The factor $\exp(\pi q)$ is really superfluous to the order of accuracy aimed at, but it is in fact more important than any other higher-order corrections. (Here $\psi(x)$ denotes the function $d/dx \ln \Gamma(x)$.)

Other known formulae can be obtained by further approximations. Thus if ξ and η are large, Re $\psi(1+iX) \sim \ln X$ and (18) goes over into (13). If on the other hand they are both small $(X \ll 1)$ one obtains $g = (\sqrt{3}/\pi) \ln [(\eta + \xi)/(\eta - \xi)]$ —the usual formula for high (but not relativistic) energies.

6. Comparison with previous work

Karzas and Latter (1960) have computed g directly from hypergeometric series for a wide range of numerical values, and have given a family of curves; we have not made any detailed comparison.

For the conditions of the main part of this paper (§ 3), Elwert has given a complicated formula (Elwert 1948, 'Voraussetzung I' equations (18) to (20)), which is inconsistent with our result (11) except in the limit, and is not a function of a single variable. The discrepancy can be traced to a point (Elwert 1939, p 187) at which he retained the first two terms of a power series in which the powers decrease rapidly, but apparently overlooked the fact that the coefficients increase just as rapidly.

Menzel and Pekeris (1935), in the course of a remarkable paper covering many topics, deal with the circumstances of our §4 and of §5. In the case of $\xi \simeq \eta$ (ξ and η finite), their result (1.49) disagrees with our (11); this is because the approximations made in reaching their (A.26) assume more severe restrictions on $\eta - \xi$. In the case when the ratio ξ/η is not near 1, they used a method which is in principle very similar to ours but is more laborious. Their result is equivalent to our (17) except for one term. The discrepancy originates in the fourth term of a complicated expansion (A.12), in which + 121/700 should be - 1/140; in consequence, the number 484/15 should be replaced by - 4/3 in (1.38)–(1.41) and elsewhere in their work.

Appendix 1

Sommerfeld and Maue (Sommerfeld and Maue 1935, Sommerfeld 1940) derived a theoretical cross section which depends on an expression of the form

$$x(d/dx)|F(-i\xi, -i\eta, 1; x)|^2$$
.

To prove that this is equivalent to our formula (2), we require an identity for hypergeometric functions.

We need not write the third and fourth variables, which are always c = 1 and $x = -4\zeta \eta/(\eta - \zeta)^2$, and we consider

$$S \equiv x(d/dx)[F(a, b)F(-a, -b)].$$

It is obvious from the hypergeometric series that

$$aF(a, b) + xF'(a, b) = aF(a+1, b).$$
 (A.1)

By making the replacements $a \rightarrow -b, b \rightarrow -a$ one obtains also

$$bF(-a, -b) - xF'(-a, -b) = bF(-a, -b+1) = (1-x)^{a+b}bF(a+1, b).$$
(A.2)

Now multiply the left-hand sides of (A.1) and (A.2); from the product subtract the same thing with a and b interchanged; and do the same to the right-hand sides. This yields the identity

$$(b-a)S = ab(1-x)^{a+b}[F(a+1,b)^2 - F(a,b+1)^2].$$

The equivalence then follows immediately.

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Appendix 2

The fact that each term in the hypergeometric series

$$F(-iX + \frac{1}{2}m, iX + \frac{1}{2}m, m; q^2/4X^2) = \sum_{s=0}^{\infty} u_s(X)$$

tends to a limit as $X \to \infty$, which was used above (at equation (7)), is obvious enough, but it is necessary to show that the convergence is uniform in some interval (X_0, ∞) ; here m is any complex constant. Now

$$\frac{u_{s+1}(X)}{u_s(X)} = \frac{X^2 + (s + \frac{1}{2}m)^2}{(s+m)(s+1)} \frac{q^2}{4X^2}$$

Let s_1 be chosen so that

$$\frac{|s+\frac{1}{2}m|^2}{|s+m|(s+1)} < 4$$

for all $s > s_1$. Then, for $s > s_1$,

$$\left|\frac{u_{s+1}(X)}{u_s(X)}\right| < \frac{\frac{1}{4}q^2}{|s+m|(s+1)} + \frac{q^2}{X^2}$$

and this will be less than $\frac{1}{2}$ for all X in the range $(2q, \infty)$ when s is also greater than some s_2 independent of X. The uniform convergence is now easily deduced.

Appendix 3

One of the standard ways (Perron 1917) of evaluating a saddle-point integral such as (15) or (16) is to express the integrand in (16) as

$$e^{\pi\xi} \exp[-\frac{2}{3}i\xi(1-\rho^2)t^3] \exp[1-\frac{2}{5}i\xi(1-\rho^4)t^5+\ldots]f(t),$$
(A.3)

combine the last two factors into a power series, and integrate along a tangent to the curve of steepest descent. By an obvious change of variable, each term in the power series gives rise to an integral of the form $\int e^{-v}v^n dv$ with v real.

It is simpler however to avoid bringing in Γ functions by using the Airy integral function (Miller 1946, Abramowitz and Stegun 1964, § 10.4). By differentiating Airy's integral(in one of the usual forms) *n* times, and then writing *kt* for the variable of integration, one obtains

$$I_n \equiv \frac{1}{2\pi i} \int_{\infty \exp(-5i\pi/6)}^{\infty \exp(-i\pi/6)} \exp(-\frac{1}{3}ik^3t^3) t^n dt = \frac{i^{n-1}}{k^{n+1}} \operatorname{Ai}^{(n)} 0.$$
(A.4)

The *n*th derivatives appearing on the right of (A.4) are found from the Taylor series

Aix =
$$A\left(1 + \frac{1}{3!}x^3 + \frac{1 \cdot 4}{6!}x^6 \dots\right) + A'\left(x + \frac{2}{4!}x^4 + \frac{2 \cdot 5}{7!}x^7 \dots\right).$$

They are:

n	0	1	2	3	4	5	6	7	8	9
Ai ⁽ⁿ⁾ 0	A	A'	0	A	2 <i>A'</i>	0	4 <i>A</i>	10 <i>A'</i>	0	28 <i>A</i>

In order to evaluate the sum and difference of the two functions in (2), f(t) in (16) must be replaced by the series expansion of $(1 - \rho^2 t^2)^{-1}(1 - t^2)^{-1}$ multiplied by $-2(1 + \rho)t$ or by $-2(1 + \rho t^2)$ respectively; one then multiplies by the series on the right of (A.3), suppressing terms in t^2 , t^5 or t^8 which yield nothing. Applying (A.4) with $k^3 = 2\xi(1 - \rho^2)$ now gives, for the sum and difference of the integrals (15), $2\pi i e^{\pi\xi}$ times

$$-\frac{2(1+\rho)}{k^2}\left[A'-\frac{1+\rho^2}{k^2}A+O\left(\frac{1}{k^6}\right)\right]$$

and

$$\frac{2i}{k} \left(A + 0 + \frac{6 - 8\rho^2 + 6\rho^4}{35k^4} A' + \ldots \right)$$

respectively. After inserting the external factors from (15) and using $AA' = -1/2\pi\sqrt{3}$ one finds the result

$$D = \frac{i e^{2\pi\xi}}{\pi(\sqrt{3})\xi\eta} \left(\frac{\eta+\xi}{\eta-\xi}\right)^{2i\xi+2i\eta} \left(1 - \frac{A}{5A'} \frac{1+\rho^2}{k^2} + \frac{2A'}{35A} \frac{3-4\rho^2+3\rho^4}{k^4} \dots\right).$$
 (A.5)

The values of A = Ai0 and A' = Ai'0 are given by Miller (1946) and Abramowitz and Stegun (1964).

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