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Zeros in (inverse) bremsstrahlung matrix elements

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Abstract

We discuss the possibility of zeros in the non-relativistic radiative continuum–continuum matrix element for electron–atom (inverse) bremsstrahlung. As earlier demonstrated for upward transitions from bound states, the occurrence of different signs for the free-free matrix element in limiting cases, plus the requirement of continuity, implies existence of zeros. Using knowledge of the sign of the dipole matrix element in the soft and hard photon limits with one continuum electron energy held fixed, we show that zeros can occur in the s–p matrix element. We discuss the connection of our results to elastic scattering and to Ramsauer-Townsend minima. We consider the observability of zeros in this (s–p) matrix element manifested as minima in the cross sections.

I. INTRODUCTION

We consider the possibility of zeros in the non-relativistic continuum–continuum dipole matrix element for radiative transitions of an electron in the static field of an atom or ion. In previous work [1,2], the existence of zeros in upward transitions from bound states was predicted by calculating the sign of such transition matrix elements in the soft and hard photon limiting cases. Using arguments for the continuity of the matrix element in energy, the existence of zeros then followed whenever the sign was different in the two limiting cases. The present work can be considered a natural extension of these arguments to the case of continuum–continuum transitions.

In Section II we examine the behavior of the dipole radial matrix element, holding one electron energy fixed, in the soft photon limit, demonstrating that the sign of the matrix element in this limit can be determined from a knowledge of the phase shifts for elastic scattering in the potential. Next we again fix one electron energy and consider the limiting case where the other electron energy is taken to infinity. Utilizing the knowledge that in this limit the radial matrix element is determined at small distances [3], the sign of the matrix element may be determined by evaluating the radial integral using Coulomb wavefunctions. From the continuity of the matrix element in energy, the existence of zeros in certain cases can then be predicted. Our results for the soft photon case are also suggestive of the intimate connection to elastic scattering phenomena. In Section III we discuss this connection and the relation of free-free zeros to Ramsauer-Townsend minima observed in elastic scattering. Finally, in Section IV we discuss the issue of observability of the predicted zero crossings in these free-free transition matrix elements.

II. ZEROS IN FREE-FREE MATRIX ELEMENTS

We begin by writing the non-relativistic dipole bremsstrahlung matrix element for a spin-less electron

$$M_{fi}^{\mathrm{nrd}} = \int \psi_2^* \left(\vec{\epsilon}^{\,*} \cdot \vec{p}\right) \psi_1 d^3 r, \tag{1}$$

where ψ_2 and ψ_1 are continuum solutions of the full three dimensional Schrödinger equation representing the initial and final states of the electron respectively, ϵ is the photon polarization vector and $\vec{p}$ is the momentum operator (as discussed, for example, in [4]). The partial wave decomposed form of this matrix element is written [4],

$$M_{fi}^{\rm nrd} = (ik/p_1p_2)\sum_m (\hat\epsilon)_m^* \sum_{l_1,m_1,l_2,m_2} \Bigg[(-1)^{l_2} i^{l_1} i^{l_2} e^{i(\delta_{l_1}+\sigma_{l_1})} e^{i(\delta_{l_2}+\sigma_{l_2})}$$
$$\times Y_{l_1,m_1}^*(\hat p_1) Y_{l_2,m_2}(\hat p_2) R_{l_1,l_2}(E_1,E_2)$$
$$\times \sqrt{\frac{3(2l_1+1)}{4\pi(2l_2+1)}} \left\langle l_1 1;00|l_1 1;l_2 0\right\rangle \left\langle l_1 1; m_1 m|l_1 1; l_2 m_2\right\rangle \Bigg], \tag{2}$$

where the ionic Coulombic phase shift

$$\sigma_l = \arg\Gamma(l+1+i\eta_{\rm ion}), \tag{3}$$

δ_l is the (energy dependent) short range phase shift, $\eta_{\rm ion} = -Z_{ion}/p$ is the Coulomb parameter corresponding to the ionic charge $Z_{\rm ion}(\eta_{\rm ion} = \sigma_l \equiv 0$ for a neutral atom), $\vec p_{1,2}$ are the electron momenta (with magnitudes $p_{1,2}$) and the unit vectors $\hat p_{1,2} = \vec p_{1,2}/p_{1,2}$), $\hat\epsilon$ is a unit vector in the direction of the photon polarization, and Y_{LM} are the spherical harmonics. [In all of our equations we use atomic units ($m = e = \hbar = 1$, m the mass of the electron, e the charge of the electron, and $\hbar$ Planck's constant divided by 2π).] In the summation in Eq. (2), m represents the z component of the angular momentum of the photon, l_1, m_1 (l_2, m_2) represent the angular momentum and its z component for the initial (final) electron. We have used the notation of [5] for the Clebsch-Gordan coefficients $\langle LL'; MM'|LL'; JM_J\rangle$ and the notation for a spherical vector $(\vec\epsilon)_m$ derived from a Cartesian vector $\vec\epsilon$ (and the corresponding unit vector $\hat\epsilon$)

$$(\vec\epsilon)_m = |\vec\epsilon|\, Y_{1m}(\hat\epsilon).$$

The bremsstrahlung cross section can then be obtained as

$$\frac{d^3\sigma}{dk d\Omega_2 d\Omega_1} = 4\pi^2\alpha k \left| M_{fi}^{\rm nrd}\right|^2,$$

where $\alpha = e^2/\hbar c$ is the fine structure constant.

The radial matrix element is written in terms of the radial wave functions as

$$R_{l_1,l_2}(E_1,E_2) = \int dr\, \phi_{l_2}(E_2;r)\, r\, \phi_{l_1}(E_1;r). \tag{4}$$

We note this radial matrix element is the same as would appear in the partial wave decomposition of the matrix element for absorption of a photon by an electron scattering from an atom or ion – inverse bremsstrahlung. Thus the considerations which follow for this matrix element also apply to the process of inverse bremsstrahlung.

The radial wavefunctions $r^{-1}\phi_l(E;r)$ which enter the radial matrix element $R_{l_1,l_2}(E_1,E_2)$ are defined as the real-valued solutions of the radial Schrödinger equation

$$\frac{d^2}{dr^2}\phi_l(E;r) - \left[\frac{l(l+1)}{r^2} + 2V(r) - 2E\right]\phi_l(E;r) = 0, \tag{5}$$

with the asymptotic forms

$$\phi_l(E;r) \to N_l \left(\frac{2}{\pi\sqrt{E}}\right)^{1/2} \sin(pr - \eta_{\rm ion}\ln 2pr - l\pi/2 + \delta_l + \sigma_l) \quad \text{as } r \to \infty, \tag{6}$$

$$\phi_l(E;r) \to r^{l+1} \quad \text{as } r \to 0. \tag{7}$$

The normalization constant N_l is chosen so that, as above, the coefficient of r^{l+1} near the origin is unity. In the Coulomb case,

$$N_l^{\rm coul} = \frac{\Gamma(2l+2)}{2^l e^{-\pi\eta/2}\left|\Gamma(l+1+i\eta)\right|}. \tag{8}$$

We require that the phase shifts δ_l and the normalization N_l be continuous functions of energy [6], as are the Coulomb normalization and phase. For most potentials the normalization constant, so defined, will not change sign as a function of energy, since an energy for which $N_l = 0$ would correspond to a bound state in the continuum [6]. Note that, since the photon carries one unit of angular momentum (through the vector $\hat{\epsilon}$), the Clebsch-Gordan coefficients in Eq. (2) are zero unless $l_2 = l_1 \pm 1$ and $m_2 = m_1 + m$, as expected in the dipole approximation.

In the following subsections we consider the radial matrix element, Eq. (4), for dipole transitions, as a function of the energies E_1 and E_2. This matrix element is a continuous function of both E_1 and E_2 (except when $E_1 = E_2$), if (as above) we suitably choose the definition of the normalizations of the wavefunctions $\phi_l(E;r)$ [7,8]. Note we have used wavefunctions (ϕ_l) normalized so that the coefficient of r^{l+1} in the expansion of $\phi_l(E;r)$ about $r=0$ is unity. Since this normalization condition is independent of E, Poincaré's theorem [6] applies and the ϕ_l are analytic in E. In this way we can be sure that $R_{l_1,l_2}(E_1,E_2)$, as defined above, is analytic except when $E_1 = E_2$ and that for E real and $E > 0$ the two limiting cases we will consider are limiting cases for R_{l_1,l_2} of the same continuous matrix element [9,8].

A. The soft photon limit

In the limit that the photon energy k goes to zero with one electron energy fixed (the soft photon limit), $R_{l_1,l_2}(E_1, E_2)$ is known to diverge as $1/k^2$ [4]. We wish to determine the sign of R_{l_1,l_2} in this limit. To obtain the leading divergent term in R_{l_1,l_2}, following Lassetre [10], we first partition the radial integral in Eq. (4) into contributions from two regions,

$$\begin{aligned}\int_0^\infty &= \int_0^{r_c} + \int_{r_c}^\infty \\ &= I_0 + I_d,\end{aligned}$$

where r_c is chosen to be sufficiently large that the wavefunctions will have reached, at least approximately [11], their asymptotic form given by Eq. (6). If we analytically evaluate the integral I_d using (6) and retain only the dominant term in the soft photon limit, we obtain

$$I_d \to N_{l_1} N_{l_2} \frac{4\sqrt{E}}{\pi} \frac{\sin \Delta_{l_1,l_2}(E)}{k^2} \text{ as } k \to 0, \tag{9}$$

where we have taken $E_1 \approx E_2 = E$. Here $\Delta_{l_1,l_2}(E) = \delta_{l_<} - \delta_{l_>} + \sigma_{l_<} - \sigma_{l_>}$, where $l_<(l_>)$ is the lesser (greater) of l_1 and l_2. In the soft photon limit, I_d diverges as $1/k^2$. Since the integrand is well behaved in the region from 0 to r_c, the integral I_0 does not give a divergent contribution (for finite r_c) even in the soft photon limit.

Thus we obtain (retaining only I_d) [12]

$$R_{l_1,l_2}(E_1, E_2) \to N_{l_1} N_{l_2} \frac{4\sqrt{E}}{\pi} \frac{\sin \Delta_{l_1,l_2}(E)}{k^2} \quad \text{as} \quad k \to 0. \tag{10}$$

We see that in the soft photon limit $R_{l_1,l_2}(E_1, E_2)$ is singular with a sign that depends upon the phase shift difference $\Delta_{l_1,l_2}(E)$ and on the signs of N_{l_1} and N_{l_2}. Whenever $\Delta_{l_1,l_2}(E)$ crosses $n\pi$, for integers n, as a function of E the matrix element in the soft photon limit passes through zero and changes sign. Examples of such crossings can be found in realistic elastic scattering phase shift calculations [13–15]. Of course, it may be possible for $\Delta_{l_1,l_2}(E)$ to become equal to $n\pi$ without crossing it. In such a case, the soft photon matrix element would have a zero but would not change sign. We do not address such phenomena explicitly here and we will be concerned with and refer to "zero crossings" throughout this paper.

In the pure Coulomb case $\Delta_{l_1,l_2}(E)$ can be written analytically, using the relation [16]

$$\arg\Gamma(z+1) = \arg\Gamma(z) + \tan^{-1}\frac{y}{x}, \tag{11}$$

where $z = x + iy$ and x and y are real and the range of the arctangent is taken to be $-\pi/2$ to $\pi/2$. Using this relation and Eq. (3) we obtain

$$\begin{aligned} \Delta^{\rm coul}_{l_1,l_2}(E) &= -\tan^{-1}\frac{\eta_{\rm ion}}{l_< + 1}, \\ &= -\sin^{-1}\left\{\frac{\eta_{\rm ion}}{l_< + 1}\left[1 + \frac{\eta^2_{\rm ion}}{(l_< + 1)^2}\right]^{-1/2}\right\}, \end{aligned} \tag{12}$$

with the range of the arcsine function taken to be $-\pi/2$ to $\pi/2$. For an attractive Coulomb potential ($\eta_{\rm ion} < 0$), we have $0 < \Delta^{\rm coul}_{l_1,l_2}(E) < \pi/2$. The Coulomb normalization is given by Eq. (8) and is always positive. Thus, in an attractive pure Coulomb potential, the matrix element in the soft photon limit $R_{l_1,l_2}(E,E)$ never changes sign. In the pure Coulomb case we obtain the soft photon result [17]

$$R^{\rm coul}_{l_1,l_2} = -\frac{4\sqrt{E}}{\pi}N_{l_1}N_{l_2}\frac{1}{k^2}\frac{\eta_{\rm ion}}{l_< + 1}\left[1 + \frac{\eta^2_{\rm ion}}{(l_< + 1)^2}\right]^{-1/2}, \tag{13}$$

which is always positive for an attractive Coulomb potential ($\eta_{\rm ion} < 0$), so that there are no soft photon zero crossings in this case. We note that in a pure Coulomb potential it has been shown [18] that, more generally, the matrix element R_{l_1,l_2} has no zeros, is always positive and is a monotonically decreasing function as one goes away from the singularity of the soft photon limit.

In a neutral or partially ionized atom, the detailed behavior of the phase shifts depends upon the potential under consideration. In general we can require [6] that $\delta_l \to 0$ as $E \to \infty$; σ_l has the same property. Thus we have

$$\Delta_{l_1,l_2}(E) \to 0 \quad \text{as } E \to \infty. \tag{14}$$

For neutral atoms, invoking Levinson's theorem [19,6], we can require that the short range phase shifts, taken to be continuous in energy [6], go to $n_l\pi$ as $E \to 0$, where n_l is the number of bound states with angular momentum l (with the exception of potentials with a *virtual* $l = 0$ bound state at threshold, sometime called a "half bound state", in which case we define n_0 as the number of actual $l = 0$ bound states plus $\frac{1}{2}$). Therefore

$$\Delta_{l_1,l_2}(E) \to (n_{l_<} - n_{l_>})\,\pi \quad \text{as } E \to 0. \tag{15}$$

For neutral atom potentials which do not support an $l = 0$ virtual bound state at threshold $R_{l_1,l_2}(E, E) \to 0$ as $E \to 0$. For such potentials, since $\Delta_{l_1,l_2}(E)$ is a continuous function of E, if $|\Delta_{l_1,l_2}(0)| > \pi$ there will be at least $|n_{l_<} - n_{l_>}| - 1$ additional zero crossings in $R_{l_1,l_2}(E, E)$ for $E > 0$ (and a zero in the limit $E \to \infty$), assuming there are no bound states in the continuum. For neutral atom potentials which do support an $l = 0$ virtual bound state at $E = 0$, the number of zero crossings for $E \geq 0$, in addition to the zero at infinite energy, is $|n_{l_<} - n_{l_>} - 1/2|$ when $|\Delta_{l_1,l_2}| \geq 3\pi/2$. For such cases the matrix element is non-zero at $E_1 = E_2 = 0$. We note that these conditions for soft photon zero crossings would force a zero in the soft photon radial matrix element. They are sufficient, but not necessary, conditions for the existence of zero crossings in the soft photon limit. In Section III we will give an example of zeros in the soft photon limit, corresponding to Ramsauer-Townsend minima in elastic scattering, which are not *required* by the arguments above.

For positive ions, we can use a generalization of Levinson's theorem [20–22] which gives the zero energy phase shifts in terms of zero energy quantum defects $\mu_l(0)$. We make the replacements

$$n_{l_>} \to \mu_{l_>}(0),$$
$$n_{l_<} \to \mu_{l_<}(0),$$

and use the result for the difference of zero energy Coulomb phase shifts, $\Delta^{\text{coul}}_{l_1,l_2}(0) = \pi/2$, from Eq. (12), to obtain instead of (15)

$$\Delta^{\rm ion}_{l_1,l_2}(0) = \left(\mu_{l_<}(0) - \mu_{l_>}(0)\right)\pi + \pi/2. \tag{16}$$

If $\left|\Delta^{\rm ion}_{l_1,l_2}(0)\right| > \pi$ then soft photon zeros (in addition to the zero for $E \to \infty$) for $E > 0$ are required in the ionic cases. Again, this condition is sufficient but not necessary. There will be a soft photon zero at $E = 0$ in the ionic case only if $\Delta^{\rm ion}_{l_1,l_2}(0) \bmod \pi = 0$. In a study of photoionization, Yang [23] gives quantum defect differences at threshold as a function of Z for all Z, showing that, for the potentials considered in his work, this condition is satisfied for many atoms. For example, at $Z = 30$ Yang finds that $\mu_0 - \mu_1 \approx 0.6$ giving $\Delta^{\rm ion}_{l_1,l_2}(0) \approx 1.1\pi$.

In this subsection we have shown that the sign of the free-free radial matrix element in the soft photon limit can be obtained from a knowledge of the elastic scattering phase shifts. We have also demonstrated that Levinson's theorem or its generalization can be applied to *deduce* the *required* existence of zero crossings in the soft photon radial matrix elements in some cases. We will show in the next subsections that sign changes in the soft photon matrix element are indications of the existence of zero crossings in the general bremsstrahlung radial matrix element $R_{l_1,l_2}(E_1,E_2)$, even away from the soft photon limit.

B. The high energy limit

We now want to determine the sign of the matrix element $R_{l_1,l_2}(E_1,E_2)$ in the limit $E_1 \to \infty$. (For convenience of notation we will discuss only the case where E_2 is fixed and E_1 varies but the same arguments apply when reversing the roles of the energies.) For large E_1, $\phi(E_1;r)$ will oscillate for $p_1 r \gg 1$. Since the other terms in the integrand of (4) are slowly varying on this scale, the important contributions to the integral occur when r is of the order of $1/p_1$, since for larger distances the integrand oscillates rapidly. The radial matrix element for fixed l in this high energy limit will be determined in this small r region. Since a realistic atomic potential would have nuclear Coulombic behavior at this length scale, it is sufficient to use wave functions $\phi_l(E;r)$ for a particle in a Coulomb potential with nuclear charge Z. That is, we can use the reduced Coulomb functions $\phi_l(E;r) = F_l(\eta;pr)$

(normalized to r^{l+1} near the origin), where $\eta = -Z/p$ is the (nuclear) Coulomb parameter. It has previously been demonstrated [24] that the dipole Coulomb free-free matrix element is positive everywhere (and thus in the high energy limit considered here). It is nevertheless useful to obtain an expression for the matrix element in this high energy limit. We may expand the wavefunction for the slow electron, $\phi_{l_2}(E_2;r)$, about $r=0$, keeping terms up to order r^{l_2+2} (the first two terms):

$$\phi_{l_2}(E_2;r) = r^{l_2+1}\left[1 + B_{l_2}(\eta_2) r\right], \tag{17}$$

where

$$B_{l_2}(\eta_2) = \frac{p_2\eta_2}{l_2+1}. \tag{18}$$

Inserting this expansion in Eq. (4), and using the Coulomb function for $\phi_l(E;r)$,we obtain

$$R_{l_1,l_2}(E_1,E_2) \to \int_0^\infty \left[r^{l_2+1} + B_{l_2}(\eta_2) r^{l_2+2}\right] r F_{l_1}(\eta_1; p_1 r)\, dr \quad \text{as} \quad E_1 \to \infty. \tag{19}$$

The first two terms in the expansion (17) are needed in (19) since they contribute to the same order in the small parameter η_2 (while further terms contribute pair-wise in higher orders in η_2 or p_2/p_1 [3,25]). The *reduced* Coulomb function F_l can be expressed in terms of the confluent hypergeometric function $M(a,b,z)$, [26]

$$F_l(\eta;z) = z^{l+1} e^{-iz} M(l+1-i\eta, 2l+2, 2iz).$$

Eq. (19) can be evaluated in a straightforward manner by using an integral representation for the confluent hypergeometric function given in [27]. Landau and Lifshitz [28] give

$$J^\nu_{\alpha\gamma} = \int_0^\infty e^{-\lambda z} z^\nu F(\alpha,\gamma,kz)\, dz \tag{20}$$

$$= \Gamma(\nu+1)\lambda^{-\nu-1} F(\alpha, \nu+1, \gamma, k/\lambda), \tag{21}$$

convergent if $\Re\nu > -1$ and $\Re\lambda > |\Re k|$. To satisfy these constraints, as is conventional in defining the bremsstrahlung matrix element, we introduce the exponential $e^{-\lambda r}$ into the integrand of Eq. (20) and take the limit $\lambda \to 0^+$ after integrating, obtaining

$$
\begin{aligned}
R_{l_1,l_2}(E_1,E_2) \to\ & p_1^{-l_2-3} p_2^{l_2+1} \Gamma(l_2+l_1+4) \\
& \times \Big[i^{-l_2-l_1-4} F(l_1+1-i\eta_1, l_2+l_1+4, 2l_1+2; 2+0i) \\
& + (l_2+l_1+5) i^{-l_2-l_1-5} B_{l_2}(\eta_2) \frac{p_2}{p_1} \\
& \quad \times F(l_1+1-i\eta_1, l_2+l_1+5, 2l_1+2; 2+0i) \Big], \qquad (22)
\end{aligned}
$$

where $F(a,b,c;z)$ is the hypergeometric function and $\Gamma(z)$ is the gamma function. Since l_1 and l_2 are both integers, these hypergeometric functions can be evaluated analytically [29]. The additional constraint $l_2 = l_1 \pm 1$ simplifies this algebraically tedious calculation. Retaining only the leading term in η_2 we obtain

$$
R_{l_1,l_1+1}(E_1,E_2) \to -2\eta_1 e^{-\eta_1 \pi} p_1^{-l_1-4} p_2^{l_1+2} \Gamma(2l_1+2) \text{ as } E_1 \to \infty, \qquad (23)
$$

for upward transitions and

$$
R_{l_1,l_1-1}(E_1,E_2) \to -4\eta_1 e^{-\eta_1 \pi} p_1^{-l_1-4} p_2^{l_1+2} \frac{\Gamma(2l_1+2)}{l_1} \text{ as } E_1 \to \infty, \qquad (24)
$$

for downward transitions. Clearly

$$
R_{l_1,l_2}(E_1,E_2) \to 0^+ \qquad \text{as } E_1 \to \infty, \qquad (25)
$$

for both upward and downward transitions. That is, the matrix element $R_{l_1,l_2}(E_1,E_2)$ is positive in the limit that $E_1 \to \infty$.

C. Zero crossings

The consequences of these results for the signs of $R_{l_1,l_2}(E_1,E_2)$ can be most easily understood by looking at the first quadrant of the schematic illustration in Figure 1. From the result for the signs in the high energy limiting case described above we see that if $R_{l_1,l_2}(E^-,E^-) < 0$ for some choice of E^-, since R_{l_1,l_2} is continuous, there must be at least one zero (or more generally, an odd number of zero crossings) along any path, confined to the first quadrant without crossing the soft photon line, connecting (E^-,E^-) to $(E_1 \to \infty, E^-)$.

Similarly, if $R_{l_1,l_2}(E^+,E^+) > 0$ then we predict an even number of zero crossings (possibly none) along such a path.

While the exact trajectory (or trajectories) in the (E_1, E_2) plane of the curve(s) of zero crossings probably requires detailed calculation, based on our previous discussion we can see that it is required that one such trajectory intersect any soft photon zero crossing. Thus a zero in the soft photon matrix element must persist in bremsstrahlung away from the soft photon limit. (How far is yet unknown; results from bound-free transitions suggest that this depends on the choice of potential and change of angular momentum in the transition [23].) Closed loops of zero crossings (or paths for which both ends extend out of the first quadrant) are allowed but paths which end in the first quadrant away from the the soft photon limit are not. We illustrate this in Figure 2.

We remember, as noted above, that Levinson's theorem for short range potentials which do not support $l = 0$ virtual bound states at threshold *requires* a sign change in the soft photon matrix element $R_{l_1,l_2}(E,E)$ for $E > 0$ if the condition $|n_{l_1} - n_{l_2}| > 1$ on the difference of the number of bound states is satisfied. Similarly, the generalization to quantum defects for ions requires a soft photon zero crossing for $E > 0$ if $|\mu_{l_<}(0) - \mu_{l_>}(0) + 1/2| \geq 1$. Thus in these cases an energy E^- where $R_{l_1,l_2}(E^-,E^-) < 0$ must exist and, since $R(E^-,\infty) > 0$, there must be zero crossings in the bremsstrahlung matrix element $R(E^-,E_2)$ for some E_2.

In the theory of bound–free transitions for a neutral atom (all states in a potential with an asymptotic ionic Latter tail) it is well known that there can be a sequence of zeros in the matrix elements for transitions between Rydberg states and the continuum. In Figure 1 we have included such a sequence (in the second quadrant) for illustrative purposes. One can anticipate a continuation of such a curve of zero matrix elements into the free-free regime for such an ionic potential.

III. RELATION TO ZEROS IN ELASTIC SCATTERING

It is well known that the soft photon region ($E_1 \approx E_2$) of bremsstrahlung is related to another atomic process – elastic scattering – through the low energy theorem [30]. Consequently the zeros in the soft photon bremsstrahlung matrix elements are related to zeros in elastic scattering. It is possible, for this soft photon region, to write the bremsstrahlung radial matrix element R_{l_1,l_2} in terms of elastic scattering amplitudes or matrix elements. This allows us to see the relationship between zeros in the matrix elements for the two processes.

The relationship between matrix elements can be obtained directly through manipulation of Eq. (10). Here we demonstrate that, as noted, it is a direct consequence of the non-relativistic form of the low energy theorem for soft photons. Low [30] obtained the first two terms of the expansion of the bremsstrahlung matrix element in powers of k, the lowest order term in the series being of order $1/k$. If we retain only this lowest order term in Low's expansion and write its non-relativistic form we obtain

$$M^{\mathrm{brem}} \to \frac{1}{k}\hat{\epsilon} \cdot (\vec{p}_1 - \vec{p}_2) M^{\mathrm{elas}} \quad \text{as } k \to 0, \tag{26}$$

where M^{elas} is the elastic scattering matrix element. We note that this expression gives a dipole photon angular distribution. That is, we did not make a dipole approximation but, as expected, when we neglect relativistic terms in the low energy theorem (of higher order in the electron velocity β), we obtain a dipole angular distribution for the emitted photon.

The matrix elements in Eq. (26) correspond to *total* matrix elements, not radial matrix elements. To obtain the corresponding relationships for the radial matrix elements we must expand M^{brem} and M^{elas} in partial waves series. The expansion of $M^{\mathrm{brem}} \equiv M^{\mathrm{nrd}}_{fi}$ can be found in Eq. (2) and we simply write down the expansion of M^{elas},

$$M^{\mathrm{elas}} = \frac{2}{\pi\sqrt{E}} \sum_{lm} f_l^{\mathrm{elas}}(p) Y_{lm}(\hat{p}_2) Y^*_{lm}(\hat{p}_1),$$

where the elastic scattering amplitudes

$$f_l^{\mathrm{elas}}(p) = \frac{e^{i(\delta_l+\sigma_l)}\sin(\delta_l+\sigma_l)}{p}. \tag{27}$$

We write the right hand side of Eq. (26)

$$M_{fi}^{\mathrm{brd}} \to \frac{2}{\pi\sqrt{E}}\frac{1}{k}\sum_m (\hat{\epsilon}^*)^*_m p\left[Y_{1m}(\hat{p}_1) - Y_{1m}(\hat{p}_2)\right]\sum_{l'm'} f_{l'}^{\mathrm{elas}}(p) Y_{l'm'}(\hat{p}_2) Y^*_{l'm'}(\hat{p}_1),$$

where the notation for the spherical vector $(\hat{\epsilon})_n$ has been used (see Section I). Note that we are not retaining terms of higher order in k; we have used $p_1 \approx p_2 \equiv p$ (for the magnitudes only!). We now utilize the orthogonality properties of the spherical harmonics,

$$\int d\Omega\, Y_{lm}(\Omega) Y^*_{l'm'}(\Omega) = \delta_{ll'}\delta_{mm'},$$

to select individual partial wave terms on both sides of Eq. (26). We obtain

$$R_{l_1,l_2} = (-1)^{l_1}\frac{4\pi p^3}{k^2} e^{-i(\delta_{l_1}+\sigma_{l_1})} e^{-i(\delta_{l_2}+\sigma_{l_2})}\left[f_{l_1}^{\mathrm{elas}} - f_{l_2}^{\mathrm{elas}}\right] \tag{28}$$

Thus R_{l_1,l_2} can be expressed in terms of the elastic scattering amplitudes for partial waves l_1 and l_2. If we insert the expressions, Eq. (27), for f_l^{elas} in terms of elastic scattering phase shifts we obtain Eq. (10).

We now discuss some features of the elastic scattering matrix elements that are, in view of the previous discussion, relevant to zeros in the bremsstrahlung matrix element. It is well known from the theory of elastic scattering that, in a short range potential at very low energy, the $l = 0$ phase shift and therefore the $l = 0$ matrix element dominates [6]. Under circumstances described in [31] it is possible that the $l = 0$ phase shift can pass through $n\pi$, $n = 0, 1, 2, ...$ in a region where it is the dominant phase shift (the potential must be sufficiently strong at small r to accommodate an integral number of wavelengths of the $l = 0$ wavefunction at energies where other phase shifts are small). This causes a zero in the dominant $l = 0$ matrix element in elastic scattering and therefore a minimum in the total elastic scattering matrix element M^{elas}. Such minima are called "Ramsauer-Townsend minima". They have been observed in experiments involving elastic scattering from noble gas atoms [31]. In Figure 3 we show the phase shifts obtained by Holtsmark [13] using a Hartree-Fock potential with an imposed long-range static dipole interaction resulting from static polarizability (see [32]). We see that at energies less than about 5 eV, the $l = 0$ phase shift is dominant, while near 2 eV it passes through 3π, causing a Ramsauer-Townsend minimum. It is also clear from this figure that (modulo π) the same phase shifts, and thus the elastic scattering amplitudes, cross near 2 eV, causing a zero and sign change in the soft photon bremsstrahlung matrix element in Eq. (28). We refer back to Figure 1 which, if we take $E^0 = 2$ eV, represents the soft photon result for Argon. In that figure we have sketched a possible trajectory of zeros, passing through this soft photon zero. From our discussion we can be assured that in cases where Ramsauer-Townsend minima occur there will also be zeros in the (s–p) bremsstrahlung matrix element away from the soft photon limit.

IV. OBSERVABILITY OF ZEROS

We now wish to address the observability of the free-free zeros we have discussed above. For bremsstrahlung many electron angular momenta, and so many transition matrix elements, begin to contribute to cross sections at energies low compared to energies considered in current experimental and theoretical efforts; they contributed at still lower energies to angular distributions. We know from elastic scattering that higher phase shifts become comparable to s–wave phase shifts by 10 eV in neutral noble gases, so observation of zeros causing Ramsauer-Townsend minima may be confined to the region near 1-10 eV. Zeros in bremsstrahlung matrix elements from neutral atoms (but less likely for ions, for which many matrix elements generally contribute at most angles) can likewise be observable when both initial and final electrons are of low energy. However, in bremsstrahlung there is additional opportunity for observation, since as long as one electron is slow, small numbers of its partial waves contribute in bremsstrahlung even as the other electron becomes fast. Whenever dipole approximation remains valid, only a few radial matrix elements are important, and one can still expect to see effects of these zeros, as in the tip region of the spectrum of faster electrons. Note that the bremsstrahlung spectrum is fairly well described in non-relativistic dipole approximation (cancellation of relativistic, retardation and higher multipole effects [33]) up toward 100 keV, so that in the tip region the s–p dipole matrix elements continue to play a dominant role in the spectrum: effects of any zeros should be visible.

Also inverse bremsstrahlung, absorption of a photon by a slow electron scattering from an atom or ion, would be a prime candidate for observation of such zeros. In many cases experiments are conducted at electron energies 1 eV $< E_1 <$ 300 eV and photon energies near the soft photon regime (typically the external field is due to CO_2 lasers with $h\nu = 0.117$ eV) [34–37]. Thus we would expect that at some electron energies the scattering electrons would be transparent to the laser in the region of the zeros discussed here.

There are several previous works which might suggest the existence of observable zeros in free-free transitions. In one calculation Zon [38] observed a deep minimum in the spectrum for absorption of a photon by low energy electrons scattering from Argon. In this work, however, Zon (appropriately) included the effects of the dynamic (rather than static) polarizability of the atom in an approximate way; it is unclear what effect this treatment has on the arguments here. Zon states that his observation is unrelated to Ramsauer-Townsend minima because the "frequency corresponding to the photoabsorption minimum is much higher in this case than the width of the Ramsauer dip." Our results here would indicate that zeros connected to Ramsauer-Townsend minima may be visible at energies away from the soft photon limit. In another investigation, Green [39,40] observed, but did not discuss, minima in transition cross sections obtained from non-relativistic dipole calculations (retaining all important dipole contributions) using wavefunctions corresponding to continuum electrons in finite temperature and density Thomas-Fermi potentials. In a third related work, Ashkin [41] compared various approximate theories to an "exact calculation" (non-relativistic but with all partial waves included) of the spectrum for absorption by electron scattering from Argon. Ashkin used the potential of Holtsmark [13], which includes a static polarizational tail and is known to produce a Ramsauer-Townsend minimum near 2 eV. His results indicated a shallow minimum in absorptivity at incident electron energies near 0.3 eV, corresponding to the outgoing electron energy of about 2 eV – far from the soft photon regime. However, this minimum is shallow enough that it is difficult to discern.

V. SUMMARY

We have demonstrated the possible existence of zeros in the bremsstrahlung matrix element by calculating the sign of this matrix element in two limiting cases – the soft photon limit, and the fast incident electron limit – and showing it need not be the same. Since the soft photon bremsstrahlung is related to elastic scattering, zeros in the soft photon bremsstrahlung are related to zeros in the elastic scattering matrix elements, in some circumstances observed as Ramsauer-Townsend minima. We have demonstrated that Levinson's theorem can be invoked to identify situations in which zeros in the soft photon radial matrix element, and therefore in the radial matrix element away from the soft photon limit, *must* exist. Similarly, we have used the extension of Levinson's theorem to the case of ionic species to identify situations where such zeros must exist in ions. We have argued that zeros in free-free matrix elements can be observable if the energy of either (or both) the incident or outgoing electron is sufficiently small.

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REFERENCES

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[1] R. H. Pratt, R. Y. Yin, and X. Liang, Phys. Rev. A **35**, 1450 (1987).

[2] Note that in [1] it is stated that the evenness or oddness of the *number* of zeros in the bound–free matrix element was determined. In fact, as with our work here, it is actually the evenness or oddness of the number of zero *crossings* that is determined. That is, it is also possible in principle to have additional zeros which are extrema of the matrix element, not corresponding to energies of a sign change.

[3] R. Y. Yin, O. V. Gabriel, and R. H. Pratt, Phys. Rev. A **36**, 1207 (1987).

[4] R. R. Johnston, J. Qual. Spec. and Rad. Trans. **7**, 815 (1967).

[5] J. J. Sakurai, in *Modern Quantum Mechanics*, edited by S. F. Tuan (Addison–Wesley, New York, 1985).

[6] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill Book Company, New York, 1966).

[7] M. A. Dillon and M. Inokuti, J. Chem. Phys. **74**, 6271 (1981).

[8] M. A. Dillon and M. Inokuti, J. Chem. Phys. **82**, 4415 (1985).

[9] E. C. Titchmarsh, *The theory of functions*, 2nd ed. (Oxford university press, London, 1939).

[10] E. N. Lassetre, J. Chem. Phys. **43**, 4479 (1965).

[11] It is possible to be more precise here. One can retain higher terms in the asymptotic expansion of the wavefunction at large distances and show that matrix elements corresponding to those terms diverge more slowly than $1/k^2$ in the soft photon limit.

[12] S. D. Oh and R. H. Pratt, “New results for bound and continuum transition matrix elements”, 1996, accepted for publication in Comments At. Mol. Phys.

[13] J. Holtsmark, Z. Phys. **55**, 437 (1929).

[14] J. Holtsmark, Z. Phys. **56**, 49 (1930).

[15] D. Thirumalai and D. G. Truhlar, Phys. Rev. A **25**, 3058 (1982).

[16] P. J. Davis, in *Handbook of Mathematical Functions*, 9th ed., edited by M. Abramowitz and I. A. Stegun (Dover Publications, Inc., New York, 1972), pp. 253–293.

[17] V. Véniard and B. Piraux, Phys. Rev. A **41**, 4019 (1990).

[18] S. D. Oh and R. H. Pratt, Phys. Rev. A **34**, 2486 (1986).

[19] L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill Book Company, New York, 1968).

[20] M. J. Seaton, C. R. Acad. Sci **240**, 1317 (1955).

[21] U. Fano and A. R. Rau, *Atomic Collisions and Spectra* (Academic, New York, 1986).

[22] L. Rosenberg, Phys. Rev. A **52**, 3824 (1995).

[23] H. W. Yang, R. H. Pratt, and X.-M. Tong (unpublished).

[24] S. D. Oh and R. H. Pratt, Phys. Rev. A **45**, 1583 (1992).

[25] R. H. Pratt, Phys. Rev. **120**, 1717 (1960).

[26] M. Abramowitz, in *Handbook of Mathematical Functions*, 9th ed., edited by M. Abramowitz and I. A. Stegun (Dover Publications, Inc., New York, 1972), pp. 537–554.

[27] L. J. Slater, in *Handbook of Mathematical Functions*, 9th ed., edited by M. Abramowitz and I. A. Stegun (Dover Publications, Inc., New York, 1972), pp. 503–535.

[28] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-relativistic Theory*, Vol. 3 of *Course of Theoretical Physics* (Pergamon Press LTD., London - Paris, 1958).

[29] F. Oberhettinger, in *Handbook of Mathematical Functions*, 9th ed., edited by M. Abramowitz and I. A. Stegun (Dover Publications, Inc., New York, 1972), pp. 555–566.

[30] F. E. Low, Phys. Rev. **110**, 974 (1958).

[31] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, Oxford, 1987), Vol. 2.

[32] H. Friedrich, *Theoretical Atomic Physics* (Springer-Verlag, New York, 1990).

[33] C. M. Lee, L. Kissel, R. H. Pratt, and H. K. Tseng, Phys. Rev. A **13**, 1714 (1976).

[34] B. Wallbank and J. K. Holmes, Phys. Rev. A **48**, R2515 (1993).

[35] A. Weingartshofer, J. K. Holmes, J. Sabbagh, and S. L. Chin, J. Phys. **B16**, 1805 (1983).

[36] B. Wallbank and J. K. Holmes, J. Phys. **B27**, 1221 (1994).

[37] D. D. Reid and J. M. Wadehra, Phys. Rev. A **50**, 4859 (1994).

[38] B. A. Zon, Sov. Phys. JETP **50**, 21 (1979).

[39] J. Green, Technical Report No. RDA-TR-4900-007, R & D Associates, Santa Monica, California (unpublished), August 1974.

[40] J. Green, Technical Report No. RDA-TR-108600-003, R & D Associates, Santa Monica, California (unpublished), September 1979.

[41] M. Ashkin, Phys. Rev. **141**, 41 (1965).

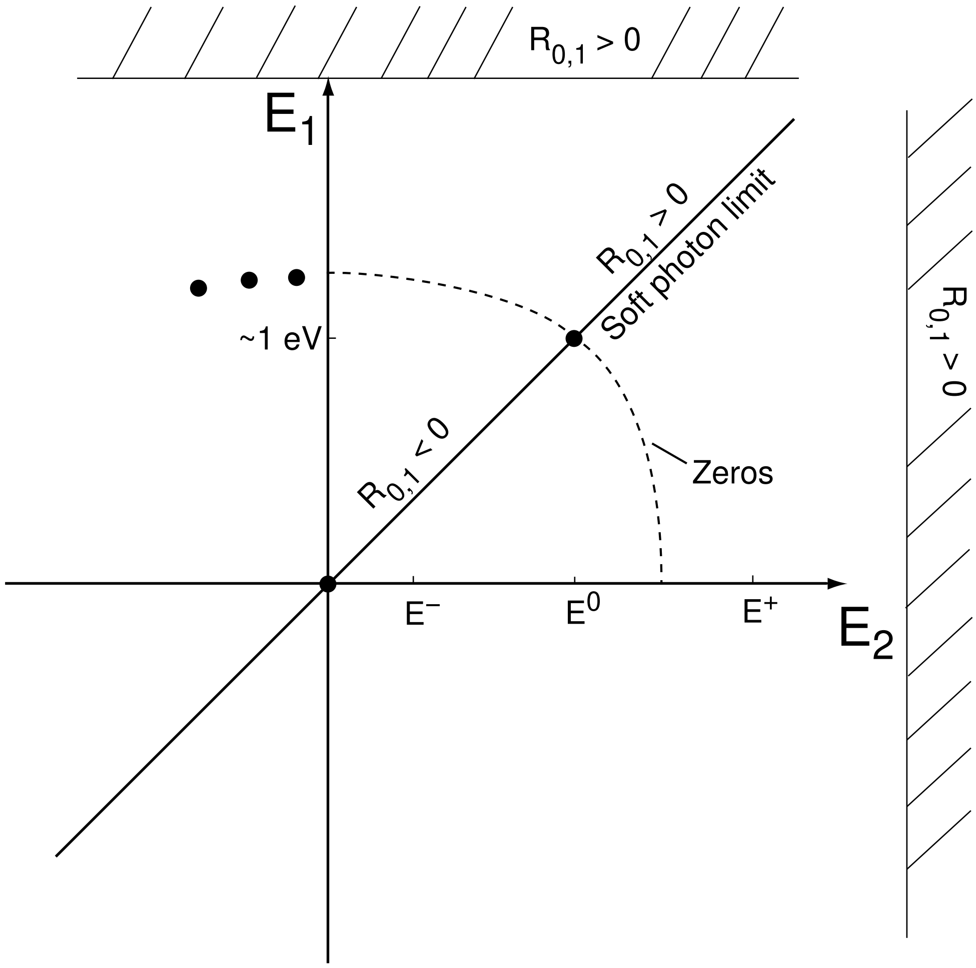

FIG. 1. Sketch of one possible trajectory of bremsstrahlung zeros based on known position of Ramsauer-Townsend minimum in elastic scattering (near E^0). The filled circle in the first quadrant represents the position of the soft photon zero associated with the Ramsauer-Townsend minimum. The filled circle at the origin represents the zero present for all neutral atom potentials which do not support $l = 0$ virtual bound states at threshold. The filled circles in the second quadrant represent the possible continuation of the bremsstrahlung zeros into the bound free transition quadrant.

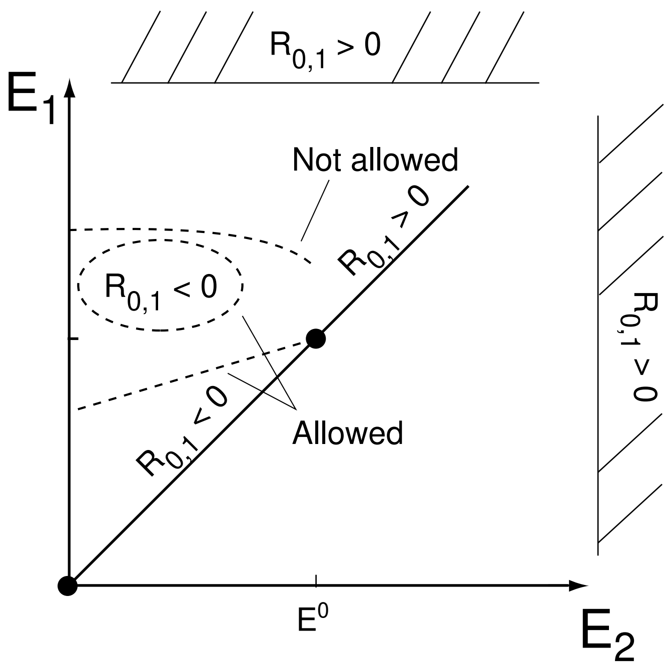

FIG. 2. Example of an allowed zero crossings trajectory and an impossible zero crossings trajectory which terminates in the first quadrant.

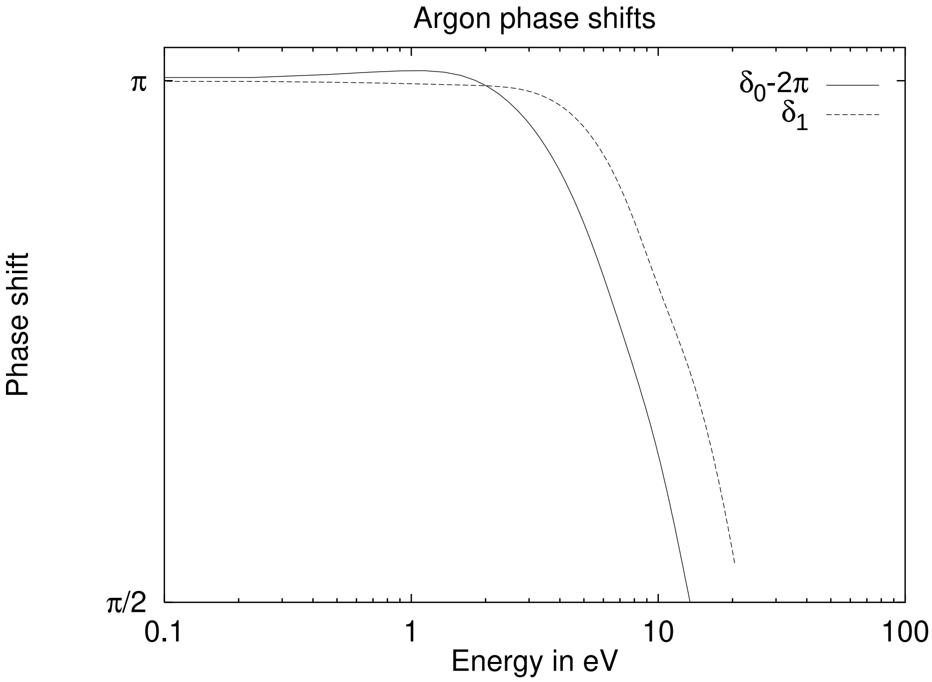

FIG. 3. A Ramsauer-Townsend minimum for scattering from neutral Argon. Plotted using numerical elastic scattering phase shifts from citeZPhys:Holtsmark29.