

Sum rules for photon scattering from bound atomic systems

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Sum rules for the forward elastic scattering of photons from bound atomic systems are obtained from the appropriate dispersion relations and the nontrivial zeros of the scattering amplitude. The significance of these sum rules for photon scattering from the hydrogenic atoms is outlined.

The problem of elastic forward photon scattering from atomic hydrogen over an extended frequency interval was first solved by Gavril.¹ Mittleman and Wolf² had earlier solved this problem for incident photon energies below the first ionization threshold. Gavril succeeded in expressing the Kramers-Heisenberg matrix element in analytic form in terms of hypergeometric functions. This work stimulated further theoretical interest on the subject of coherent forward scattering from atomic hydrogen.³⁻⁷ In this note, the elastic photon scattering from bound atomic systems, in particular the hydrogenic atoms, is considered, with a view to pointing out some sum rules which may be obtained on the basis of Gavril's calculations and by employing the dispersion relations for forward photon scattering. Sum rules of dispersion theoretic origin for photon scattering, have been discussed for some time.⁸⁻¹¹ There has been renewed interest in the search for additional sum rules which has, however, been restricted to the very-high-energy region.¹²⁻¹⁴

The basic equation relating the coherent forward scattering amplitude $r_0 f(k)$ (r_0 is the classical radius of the electron) and the total cross section is the well-known Kramers-Kronig dispersion relation

$$f_R(k) = \frac{k^2}{2\pi^2 r_0} P \int_0^\infty \frac{\sigma_T(k') dk'}{k'^2 - k^2}, \quad (1)$$

derived under the assumption that $f(k)/k$ vanishes at infinity, $f(0) = 0$, and $f(-k) = f^*(k)$. Subscripts R and I on the scattering amplitude indicate real and imaginary parts, respectively, and P stands for the principal value. Some fairly interesting sum rules may be obtained from Eq. (1) by examining the possibility that $f(k)$ has nontrivial zeros, i.e., $f(k_i) = 0$ for some $k = k_i$, where $k_i \neq 0$. If we assume the existence of one such value, denoted k_1 , then the result

$$r_0^{-1} \int_0^\infty k_1^2 (k^2 - k_1^2)^{-1} \sigma_T(k) dk = 0, \quad (2)$$

follows directly from Eq. (1). For the particular

case where several nontrivial zeros may exist, additional sum rules may be obtained. Given the subtracted dispersion relation Eq. (3)

$$f_R(k) - f_R(k_0) = (k - k_0) \frac{P}{\pi} \int_{-\infty}^\infty \frac{f_I(k') dk'}{(k' - k)(k' - k_0)}, \quad (3)$$

and designating any two nontrivial zeros as occurring at k_1, k_2 ; $f(k_1) = f(k_2) = 0$, then the following sum rule is readily obtained

$$r_0^{-1} \int_0^\infty k_1 k_2 k^2 (k^2 - k_1^2)^{-1} (k^2 - k_2^2)^{-1} \sigma_T(k) dk = 0. \quad (4)$$

The sum rule emerges independent of the subtraction at $k = k_0$. Equation (4) may of course be derived directly from Eq. (2). The constant factor $k_1 k_2$ has been explicitly included to emphasize that we exclude nontrivial zeros. Similarly, for the case of three nontrivial zeros

$$r_0^{-1} \int_0^\infty \frac{k^4 (k^2 - k_2 k_3) + k^2 k_1^2 (k_2 k_3 - k_2^2 - k_3^2) + k_1^2 k_2^2 k_3^2}{(k^2 - k_1^2)(k^2 - k_2^2)(k^2 - k_3^2)} \times \sigma_T(k) dk = 0. \quad (5)$$

A further sequence of sum rules may be obtained depending on the number of known zeros of $f(k)$. These sum rules may be collectively written down in condensed form as

$$\begin{aligned} \int_0^\infty \sigma_T(k) dk &= \int_0^\infty \frac{\sigma_T(k) k^2 dk}{k^2 - k_1^2} \\ &= \int_0^\infty \frac{\sigma_T(k) k^2 dk}{k^2 - k_2^2} = \dots \end{aligned} \quad (6)$$

A sum rule similar to Eq. (2) may be derived for the differential elastic cross section

$$r_0^{-2} \frac{d\sigma_E(k)}{d\Omega} = f_R^2(k) + f_I^2(k). \quad (7)$$

Considering the dispersion relation based on $f^2(k)/k^2$ leads to the result

$$8\pi^2 \int_0^\infty \frac{dk}{k^2(k^2 - k_1^2)} \frac{d\sigma_E(k)}{d\Omega} = \int_0^\infty \frac{\sigma_T^2(k) dk}{k^2 - k_1^2}, \quad (8)$$

where $f(k)/k \rightarrow 0$ as $k \rightarrow 0$ (the differential cross section vanishes as k^4) and k_1 is a zero of $f(k)$. An additional dispersion relation is obtained by assuming $F(k) \rightarrow 0$ as $k \rightarrow \infty$ where $F(k)$ is defined as

$$F(k) = [f^2(k) - f_R^2(k)]/k^2. \quad (9)$$

The dispersion relation based on $F(k)$ is given by

$$f_I(k)f_R(k) = \frac{k^3}{\pi} P \int_0^\infty \frac{f_I^2(k') dk'}{k'^2(k'^2 - k^2)}, \quad (10)$$

where we have used $F(k) \rightarrow 0$ as $k \rightarrow 0$ [since $f_I(k)$ is zero for $k \rightarrow 0$ and $f_R(k)$ vanishes like k^2]. Equation (10), under the assumption that a zero exists at $k = k_1$, leads to the following sum rule:

$$r_0^{-2} \int_0^\infty k_1^3(k^2 - k_1^2)^{-1} \sigma_T^2(k) dk = 0, \quad (11)$$

and hence a sum rule for the forward elastic differential scattering cross section follows directly from Eq. (8)

$$r_0^{-2} \int_0^\infty k_1^3 [k^2(k^2 - k_1^2)]^{-1} \frac{d\sigma_E(k)}{d\Omega} dk = 0. \quad (12)$$

The principal value of the integral in the above sum rules is not required since the integrands are well behaved as $k \rightarrow k_1$. This can be explicitly demonstrated from the data¹ for the hydrogen atom.

The basis of all these dispersion sum rules is the connection between $\sigma_T(k)$ and $f_I(k)$ via the optical theorem. Invariably only approximate relationships for $f(k)$ (in various powers of e) can be obtained, and the optical theorem is no longer exact. However a set of optical theorems of various orders of e^2 may be easily written, i.e., $\sigma_T^{(1)}(k)$

$= 4\pi k^{-1} r_0 f_I^{(1)}(k)$. From the point of discussing Gavril's results, $\sigma_T(k)$ is given to order e^2 and the Rayleigh differential cross section is of order e^4 . The zeros of $f(k)$ are to order e^2 . Gavril's analysis¹ needs to be supplemented by a small imaginary part in the vicinity of the p -symmetry resonances; otherwise $\sigma_T(k)$ is zero to order e^2 below the ionization threshold. In introducing such resonance structure, it is implicitly assumed that the line shapes are sufficiently narrow so as not to interfere appreciably with the results found by Gavril. This is of course entirely reasonable for the first few resonances, however very near to the threshold, this would not be true.

Gavril's calculations for the elastic scattering of photons by a hydrogen atom in the ground state have been calculated in the dipole approximation. The first three zeros are found to be located at $k = 0.859075, 0.926875$ and 0.954935 Ry. In fact below the ionization threshold, there are zeros between every two consecutive resonances of p symmetry. There are no zeros above threshold. Although scattering from the hydrogen atom exhibits zeros in the scattering amplitude (to order e^2), the functional form obtained by Gavril is unsatisfactory from the point of view of testing the above sum rules. This derives from the fact that there are an infinite number of bound-state resonances. Further, the formulation of Gavril has paid no attention to the details at resonance.⁵ So in order to test for example the sum rule for the forward elastic differential cross section, Eq. (12), it is necessary to supplement Gavril's formula by furnishing the details at each resonance; i.e., each resonant line width must be known. The above sum rules would likely be more useful for checking approximations to the scattering cross sections.

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