Singular Behavior in Electron-Atom Scattering at Small Momentum Transfer

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At fixed energy, the electron-atom differential cross section is commonly believed to be an analytic function of the momentum transfer squared K^2 around $K^2 = 0$. We negate this by demonstrating the presence of *nonanalytic* terms of the form $\sqrt{K^2}$ coming from second-order long-range terms. This result, combined with a Regge pole representation, yields a new generalized Lassettre expansion to evaluate optical oscillator strengths through the extrapolation of apparent generalized oscillator strengths to $K^2 = 0$. Electron-H scattering demonstrates our new formula over a wide range of impact energies. [S0031-9007(98)06736-2]

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In electron-atom scattering, absolute differential cross sections (DCSs) are difficult to obtain from relative measurements [1]. For optically allowed transitions, one of the most used techniques consists of extrapolating the experimental data down to zero momentum transfer. However, for these transitions, $K^2 = 0$ is unphysical and corresponds to a purely imaginary scattering angle at any finite energy E of the incoming electron. Therefore, this extrapolation relies heavily on the known behavior of the DCS near $K^2 = 0$ at finite E.

Because of the presence of an unphysical pole, the inelastic DCS becomes infinite at $K^2 = 0$. To remove this pole, the apparent generalized oscillator strength (AGOS) is introduced:

$$\mathrm{AGOS}(E, K^2) = \frac{\omega}{2} \frac{k_i}{k_f} K^2 \frac{d\sigma}{d\Omega} (E, K^2), \qquad (1)$$

where ω is the excitation energy, and k_i and k_f are the initial and final momenta of the electron, respectively. The limit of the AGOS as $K^2 \to 0$ is the optical oscillator strength (OOS),

$$\mathrm{OOS} = \lim_{K^2 \to 0} \mathrm{AGOS}(E, K^2). \qquad (2)$$

Absolute OOSs can be measured and therefore will fix the absolute scale of the DCSs through Eq. (1) for all energies. The striking and crucial result of Lassettre *et al.* [2] is that, while the AGOS is energy dependent, the OOS is not. This result, commonly known as the "Lassettre limit theorem," permits the estimation of the confidence of the extrapolated AGOS. By extrapolating the AGOS at different energies, and comparing the results, one can get a very good estimate of the real precision of both the experimental data and the extrapolation procedure.

To achieve the maximum precision of the OOS, experimentalists tend to use as high energies as possible with the smallest possible scattering angles. In this way, they attempt to reduce as much as possible the challenging "unphysical extrapolation" that involves imaginary scattering angles. Experimentally, reaching very small scattering angles may increase significantly the experimental errors [3]. Theoretically, the presence of a singularity in the AGOS that is not taken into account in the present state of the art, at $K^2 = 0$, can definitely worsen the situation when using very small K^2, and the second-order long-range terms are not negligible, as will be demonstrated in this paper.

First, consider a typical example of a standard extrapolation procedure carried out for optically allowed transitions at a few hundred eV. For such a case, one introduces the ordinary Lassettre expansion [2] (we drop the energy dependence of all the coefficients for clarity):

$$\mathrm{AGOS}(K^2) = \frac{1}{(1+x)^6} \left[f_0 + f_1 \frac{x}{(1+x)} + f_2 \frac{x^2}{(1+x)^2} + f_3 \frac{x^3}{(1+x)^3} + \dots \right], \qquad (3)$$

where

$$x = \frac{K^2}{K_L^2}, \qquad K_L^2 = [\sqrt{2I} + \sqrt{2(I-\omega)}]^2, \qquad (4)$$

with I and ω being the ionization and the excitation energies, respectively, of the atom under consideration. Following Lassettre and different authors [4], the expansion of Eq. (3) is supposed to converge in the neighborhood of $x = 0$, typically for $x < 1$. For the typical example of the excited $J = 3/2$ state of Xe at 100 eV [5] the coefficients f_i are

$$f_0 = 0.222, \qquad f_1 = -1.204, \qquad f_2 = -3.980, \qquad f_3 = 30.49; \qquad (5)$$

the f_i's are experimental fitting parameters. One immediately notices that the successive terms of this supposed "convergent" series increase dramatically; some of the terms being roughly 1 order of magnitude larger than the previous. Clearly, the series suffers from poor convergence. In this Letter we show the presence of terms in $\sqrt{x}$ in the expansion near $x = 0$ of the scattering amplitude. The apparent GOS cannot, at a given fixed impact energy,

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be expanded in a power series of x, because of the presence of nonexpandable terms in $\sqrt{x}$. The consequences of this fact are not innocent at all. Most of the noise and quantum fluctuation contributions will be picked up by the higher-order f_3 coefficient. Also, the values of the coefficients for the same resonant state but, at 500 eV [5], are

$$f_0 = 0.222, \qquad f_1 = -1.374, \qquad f_2 = 1.484, \qquad f_3 = 3.665\,. \tag{6}$$

In this case, the coefficients do not grow as fast as those at lower E. As will be seen, this is mainly because the second-order long-range terms are much smaller at this higher energy. Nevertheless, the series certainly cannot be termed as convergent. The aim of this Letter is to demonstrate the causes of these divergences and propose a new generalized Lassettre representation that will take care of them.

Second, we now come to the root of our paper, viz., the presence of a singularity at $x = 0$ (remember $x = \frac{K^2}{K_L^2}$) in the DCS, which is a $\sqrt{x}$ singularity coming from the *second-order effective potential*. This follows from Huo [6], "In exchange scattering associated with bound-bound transitions, the second-order potential has a longer range than the first order and may be important at small scattering angle." In fact, the first-order potential has a finite range (exponential decrease at large distances) and therefore produces an analytic behavior of the cross section at small K^2, just like the direct terms. This is contrary to the second-order potential that has an infinite range (it decreases the same as the inverse fourth power of the distance) and produces the $\sqrt{K^2}$ singularities. Before going into the details of the mechanism that produces these unexpected singularities, the following extremely simple paradigmatic example will shed the necessary light on this delicate matter.

Let us represent the direct and first-order exchange effective potentials by a symbolic fast decreasing exponential potential as

$$V_1(r) = C_1 e^{-\mu r} \tag{7}$$

and the second-order long-range effective potential by a symbolic slow decreasing r^{-2} potential (the physical one that decreases the same as r^{-4} will be analyzed later) as

$$V_2 = \frac{C_2}{r^2}\,. \tag{8}$$

The corresponding amplitudes are the Fourier transform of Eqs. (7) and (8) and are

$$T_1 = 4\pi \int_0^{+\infty} \frac{\sin Kr}{Kr}\, C_1 e^{-\mu r} r^2 dr = \frac{8\pi\mu C_1}{(K^2 + \mu^2)^2} \tag{9}$$

and

$$T_2 = 4\pi \int_0^{+\infty} \frac{\sin Kr}{Kr}\, \frac{C_2}{r^2}\, r^2 dr\,. \tag{10}$$

Noting that

$$\int_0^{+\infty} \frac{\sin Kr}{r}\, dr = +\pi \quad \text{if } K > 0$$
$$= -\pi \quad \text{if } K < 0\,, \tag{11}$$

we get

$$T_2 = \frac{4\pi^2 C_2}{\sqrt{K^2}}\,. \tag{12}$$

We note that Eq. (9) is a perfect analytic function of K^2 near $K^2 = 0$, as it should be, and that long-range potentials introduce nonanalytic contributions, Eq. (12), into the scattering amplitude at small momentum transfer. This is a general feature of any long-range potential. More generally, a potential decreasing the same as r^{-2n} will produce an amplitude that is only $(n - 2)$ times differentiable in the variable K^2 near $K^2 = 0$. All higher-order derivatives do not exist. From this example, one concludes that beyond the expected behavior of the scattering amplitude at small K^2,

$$T_1 = t_{10} + t_{11}K^2 + t_{12}(K^2)^2 + \ldots, \tag{13}$$

there is an unexpected behavior of the form

$$T_2 = t_{20} + t_{21}\sqrt{K^2} + \ldots. \tag{14}$$

For the realistic second-order effective long-range potential that behaves like the inverse fourth power of the distance at large distances, we can model it by

$$V_2(r) = \frac{C_2}{r^4 + \alpha^4}\,. \tag{15}$$

The corresponding amplitude is

$$T_2 = 4\pi \int_0^{+\infty} \frac{\sin Kr}{Kr}\, \frac{C_2}{r^4 + \alpha^4}\, r^2 dr \tag{16}$$

which, after a simple integration in the complex plane, reduces to

$$T_2 = \frac{\pi^2 C_2}{\alpha\sqrt{2}}\, e^{-\alpha\sqrt{K^2/2}}\, \frac{\sin\left(\alpha\sqrt{\frac{K^2}{2}}\right)}{\alpha\sqrt{\frac{K^2}{2}}}\,. \tag{17}$$

To clarify the content of Eq. (17) near $K^2 = 0$, let us expand it:

$$T_2 = \frac{\pi^2 C_2}{\alpha\sqrt{2}}\left(1 - \alpha\sqrt{\frac{K^2}{2}} + \frac{\alpha^2}{6}K^2 + \ldots\right). \tag{18}$$

Equation (18) clearly shows the presence of nonanalytic terms in K^2 near $K^2 = 0$. Consequently, the AGOS should be expanded in a formal series of the variable

$$\xi = \frac{\frac{K}{K_L}}{\sqrt{1 + \left(\frac{K}{K_L}\right)^2}}\,. \tag{19}$$

The crux of the argument for expanding the AGOS in powers of ξ and not of ξ^2 is that the newly proposed expansion of the AGOS keeps both odd and even powers of K. This "parity mixing" is due to the lack of analyticity of the AGOS near $K^2 = 0$. To understand this mechanism that is not at all obvious, we give a very simple paradigmatic example which contains all the essence of the process without complexity.

Suppose the DCS is given by

$$\frac{d\sigma}{d\Omega} = \frac{\text{OOS}}{K^2} + A\sqrt{1 + \frac{K_L^2}{K^2}} + B\sqrt{1 + \frac{K^2}{K_L^2}}, \quad (20)$$

where K_L^2 is the usual Lassettre unit in which the square of the momentum transfer is measured. This is a perfectly decent parity invariant function that is even in K. The AGOS, up to a constant, is given by

$$\text{AGOS} = \text{OOS} + AK^2\sqrt{1 + \frac{K_L^2}{K^2}} + BK^2\sqrt{1 + \frac{K^2}{K_L^2}}. \quad (21)$$

This again is a perfectly decent parity invariant function that is even in K. Let us now look at the small K expansion behavior. We get

$$\text{AGOS} = \text{OOS} + AK + BK^2 + \dots, \quad (22)$$

where we have written the expansion in small positive K.

Now, if we analytically continue this expansion to complex values of K and, in particular, to negative ones, we discover that we have a parity mixing. There is now a mixture of even and odd powers of K. This phenomenon can be related to the classical "Stokes phenomenon" [7] that may occur when expanding an analytical function near a singular point.

What about the convergence of the new series in the variable ξ? At least, we proved that *formally* the series exists, viz., the AGOS has derivatives of all orders in $K = \sqrt{K^2}$ when taking the limit coming from positive values of K. The most optimistic situation would be that the series is an asymptotic series with an anti-Stokes line along the real axis. The series could behave as an "effective" convergent series up to a number of terms that increases with increasing energy. The full analysis of such a structure requires the study of the delicate convergence of the Born series and will be the subject of forthcoming papers.

The second part of this Letter combines the previous result with the very efficient Regge pole approach [8], where only the direct terms were taken into account. In the present case, where we analyze a K^2 region before the first minimum, we can neglect the imaginary part of the leading Regge pole (that controls the oscillations in the DCS) and write the following generalized Lassettre formula (with only one Regge pole):

$$\text{AGOS}(E, K^2) = \frac{\text{OOS}}{(1 + x)^6} + A\,\frac{\omega}{E}\,\frac{\sqrt{x}}{(1 + x)^{\nu(E)}}, \quad (23)$$

where the OOS and A do not depend on energy and

$$\nu(E) = 6 + \frac{C}{\frac{E}{\omega}\ln\frac{E}{\omega}}. \quad (24)$$

Equation (24) can be derived by computing the next-order term in the expansion (8-4), page 62, of Ref. [9]. The constant C could be computed knowing the behavior at small distances of the corresponding effective potential.

Equations (23) and (24) give a *global analysis* of the AGOS in terms of *only three* energy independent parameters A, C, and OOS. To demonstrate the dramatic improvement that this new analysis introduces, we consider a realistic case where it is possible to separate, in the evaluation of the OOS, the limit of the AGOS as $K^2 \to 0$, the effect, on the final precision, of the interpolation procedure, the experimental errors, and quantum fluctuations. For the electron excitation H $1s$-$2p$, the OOS is known theoretically and reliable theoretical calculations [10] exist. We use the results of [10] at 35, 40, 54.4, 100, and 200 eV and scattering angles from zero to 90° for the illustration.

We first perform a fixed energy analysis using only Eq. (23) and compare the precision obtained for the OOS when the energy varies from 35 to 200 eV with values from the corresponding standard Lassettre expansion. Then a global analysis is effected by combining Eqs. (23) and (24). The results are compared in Table I.

The first striking fact in Table I is the outstanding OOS values accomplished by the Regge approach even at low energies. At 35 eV, for example, the OOS (with only a three parameter fit) is within a 2.2% error of the exact; this can be contrasted with the 23.2% error from the standard Lassettre analysis. The second important point is the use, for the first time, of a *global* approach that involves simultaneously all energies and all scattering angles (less than 90°) to extract the OOS within less than 1% with only three parameters (including the unknown OOS itself). A total of 75 data points were used (15 angles for each of the 5 energies). Finally, the 75 data are globally reproduced within a few percent with $C = 12.2$ and $A = -2.98$. The exceptional results confirm the physical content of the Regge pole approach which should become the new formalism for medium to high energy electron-atom scattering. The theoretical calculation of the two parameters C and A is in progress.

TABLE I. Extrapolated OOSs for the H $1s$-$2p$ transition.

Energy (eV)	Regge pole extrapolated OOSs	Lassettre extrapolated OOSs	% error using Lassettre	% error using Regge
35	0.4072	0.3198	23.2	2.2
40	0.4112	0.3341	19.8	1.3
54.4	0.4115	0.3593	13.8	1.2
100	0.4122	0.3885	6.7	1.03
200	0.4124	0.4040	3	0.98
Global	0.4129	N.A.	N.A.	0.86

Finally, the Regge pole formalism will henceforth be extended to electron-ion scattering and will be used immediately in the normalization of measured relative electron DCSs [11].

The experimental investigation of Eq. (23) using electron and positron projectiles on suitable atomic targets may reveal the exchange component of the second-order long-range potential.

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[1] T. Ester and J. Kessler, J. Phys. B **27**, 4295 (1994).
[2] E. N. Lassettre, A. Skerbele, and M. A. Dillon, J. Chem. Phys. **50**, 1829 (1969).
[3] C. C. Turci, J. T. Francis, T. Tyliszczak, G. G. B. de Souza, and A. P. Hitchcock, Phys. Rev. A **52**, 4678 (1995).
[4] K. N. Klump and E. N. Lassettre, J. Chem. Phys. **68**, 886 (1978); D. Bessis, A. Haffad, and A. Z. Msezane, Phys. Rev. A **49**, 3366 (1994).
[5] T. Y. Suzuki, Y. Sakai, B. S. Min, T. Takayanagi, K. Wakiya, H. Suzuki, T. Inaba, and H. Takuma, Phys. Rev. A **43**, 5867 (1991), and references therein.
[6] W. M. Huo, J. Chem. Phys. **60**, 3544 (1974).
[7] A. K. Immink, SIAM J. Math. Anal. **22**, 524–542 (1991).
[8] A. Haffad, Z. Felfli, A. Z. Msezane, and D. Bessis, Phys. Rev. Lett. **76**, 2456 (1996); V. De Alfaro and T. Regge, *Potential Scattering* (North-Holland, Amsterdam, 1965).
[9] R. G. Newton, *The Complex j-Plane* (Benjamin, New York, 1964).
[10] I. Bray, D. A. Konovalov, and I. E. McCarthy, Phys. Rev. A **44**, 5586 (1991).
[11] Z. Felfli and A. Z. Msezane, J. Phys. B **31**, L165 (1998).