Universal formula to extrapolate the generalized oscillator strength through the unphysical region to $K^2=0$

Alfred Z. Msezane and I. A. Sakmar
Department of Physics, Clark Atlanta University, Atlanta, Georgia 30314
and Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia 30314
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Rigorous bounds are derived for the momentum-transfer squared, K^2, and used to construct a universal formula to extrapolate the generalized oscillator strength through the unphysical region to the optical oscillator strength. Results of the universal function are compared with those obtained from experimental small-angle differential cross sections to determine the range of its applicability.

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I. INTRODUCTION

Lassettre, Skerbele, and Dillon [1] have deduced that the generalized oscillator strength (GOS) converges to the optical oscillator strength f^0 as the momentum-transfer squared, $K^2 \rightarrow 0$, regardless of whether the Born approximation is valid or not, i.e., at any impact energy. The implications of Lassettre's theorem are much deeper than Bethe's result, which is valid only in the framework of the Born approximation. The limiting behavior of the GOS as $K^2 \rightarrow 0$ is important in the normalization of the experimentally determined relative differential cross sections for excitation of atoms by electron impact [2–5], calculation of cross sections for energy transfer [6], and in the determination of the optical oscillator strengths [7]. The limiting behavior of the GOS as $K^2 \rightarrow 0$ has been examined [5–10] with no clear departure from the limit theorem. However, difficulties [10] and incompatibility [11] with the limit theorem have been reported. The separation of GOS curves for Hg with different values of the kinetic energy near $K^2=0$ has been interpreted [12,13] as a manifestation of the failure of the Born approximation.

For finite electron impact energy E the value $K^2=0$ is unphysical. Therefore, it is necessary to use an interpolation-extrapolation algorithm on the experimental data to access this limit. To this end the Lassettre formula [1], which has been constructed through some modeling and/or intuition, has been used extensively. Nobody has an analytic, theoretically derived expression to extrapolate the GOS through the unphysical region to $K^2=0$. Our interest is to construct a universal extrapolation formula which is valid in the limit $K^2 \rightarrow 0$ regardless of electron-impact energy.

In this paper we have first derived rigorous bounds on K^2 and then used them to construct a universal formula to extrapolate the GOS for optically allowed transitions through the unphysical region to the optical oscillator strength. The dipole allowed transitions Kr $4p^6 \rightarrow 4p^5(^2P_{3/2})5s$ at 300 and 500 eV and Mg II $3s \rightarrow 3p$ at 50 eV are used to demonstrate the limiting behavior of our universal function through comparison with the values obtained from experimental small-angle differential cross sections. From the comparison the range of validity of the universal function is thus determined. Also, the Xe $5p^6 \rightarrow 5p^5(^2P_{3/2})6s$ dipole allowed transition is used to illustrate the general behavior of the universal function and to demonstrate the validity of the Lassettre limit theorem, regardless of impact energy.

In Sec. II we present the theory. Section III gives the results while Sec. IV deals with the discussion and conclusion.

II. THEORY

The GOS, $f_{0n}^G(K)$, is given in terms of the Born differential cross section by [14,15]

$$f_{0n}^G(K)=\frac{\omega}{2}\frac{k_0}{k_n}K^2\left(\frac{d\sigma}{d\Omega}\right)_{0n}^B , \tag{1}$$

where, in atomic units,

$$K^2=2E\left[2-\frac{\omega}{E}-2\sqrt{(1-\omega/E)}\cos\theta\right] . \tag{2}$$

ω, k_0, and k_n are, respectively, the excitation energy and the electron momenta before and after collision; K and θ are the momentum transfer and the scattering angle; and E is the total energy of the system.

Where the Born approximation is applicable, $f_{0n}^G(K)$ does not depend on E; there are pairs of E and θ, $(E_1,\theta_1;E_2,\theta_2)$, say, which belong to the same K^2. Denote $x^2=1-\omega/E$ with $\omega<E$ so that

$$E_1\left[2-\frac{\omega}{E_1}-2x_1\cos\theta_1\right]=E_2\left[2-\frac{\omega}{E_2}-2x_2\cos\theta_2\right] . \tag{3}$$

Representing $u_1=x_1\cos\theta_1$, $u_2=x_2\cos\theta_2$, and $E=\omega/(1-x^2)$, Eq. (3) then becomes

$$\frac{\omega}{1-x_1^2}(1-u_1)=\frac{\omega}{1-x_2^2}(1-u_2) , \tag{4}$$

which reduces to

$$u_1+x_2^2(1-u_1)=u_2(1-x_1^2)+x_1^2 . \tag{5}$$

Given u_1, x_1, and, say, x_2 we can find u_2. From Eq. (5) we have

$$u_2=\frac{u_1+x_2^2(1-u_1)-x_1^2}{1-x_1^2}=x_2\cos\theta_2 ,$$

with $x_1=\sqrt{1-\omega/E_1}>0$ and $x_2=\sqrt{1-\omega/E_2}>0$. Hence

$$\frac{u_1+x_2^2(1-u_1)-x_1^2}{x_2(1-x_1^{2)}}=\cos\theta_2 .$$

But $-1\le\cos\theta_2\le 1$ so that

$$-1\le\frac{u_1+x_2^2(1-u_1)-x_1^2}{x_2(1-x_1^2)}\le 1 . \quad (6)$$

In Eq. (6) $x_2(1-x_1^2)>0$ because $x_1^2=1-\omega/E<1$ and $1-\omega/E>0$. The right-hand side inequality in Eq. (6) reduces to

$$x_2=\frac{(1-x_1^2)\pm\sqrt{(1-x_1^2)^2-4(u_1-x_1^2)(1-u_1)}}{2(1-u_1)} . \quad (7)$$

Define

$$\begin{aligned}D&=(1-x_1^2)^2-4(u_1-x_1^2)(1-u_1)\\&=(1+x_1^2)^2-4u_1(1-u_1+x_1^2)\\&=[2u_1-(1+x_1^2)]^2\ge 0 \text{ (always)}\end{aligned}$$

so that Eq. (7) becomes

$$x_2=\begin{cases}\dfrac{x_1(\cos\theta_1-x_1)}{1-x_1\cos\theta_1}\equiv X_{21}\\ 1\equiv X_{22} .\end{cases} \quad (8)$$

Thus $x_2^2(1-u_1)-x_2(1-x_1^2)+u_1-x_1^2\le 0$ if x_2 is between the roots 1 and

$$-\frac{x_1^2-x_1\cos\theta_1}{1-x_1\cos\theta_1} .$$

The second inequality in Eq. (6) gives

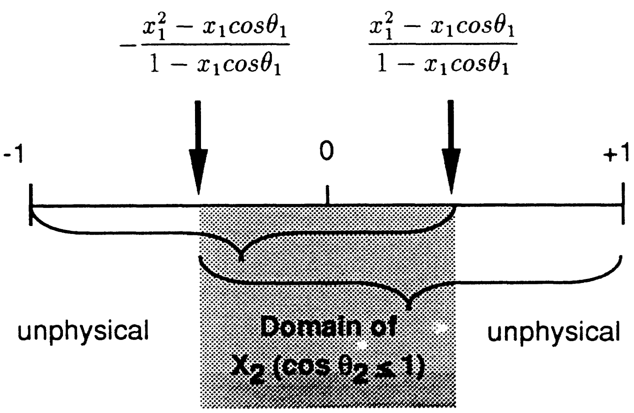
$$u_1+x_2^2(1-u_1)-x_1^2\ge -x_2(1-x_1^2) ,$$

which reduces to

$$x_2=\begin{cases}-1\equiv X'_{21}\\ \dfrac{x_1(x_1-\cos\theta_1)}{1-x_1\cos\theta_1}\equiv X'_{22} .\end{cases} \quad (9)$$

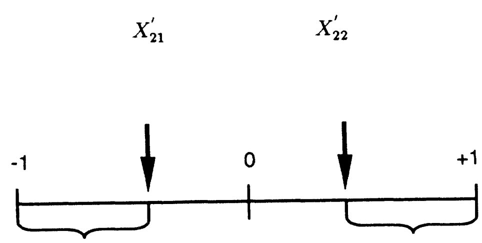
Again if $x_1>\cos\theta_1$, $X'_{22}>0$ and if $x_1<\cos\theta_1$, $X'_{22}<0$. Thus if only $x_1>\cos\theta_1$, viz., $x_1=\sqrt{1-\omega/E_1}>\cos\theta_1$ both inequalities in Eq. (6) can be satisfied.

Case A. $x_1>\cos\theta_1$:



Note that when $E_1\to\infty$, $\omega/E_1\to 0$ and $x_1\to 1$ so that the domain of x_2 is $-1\le x_2\le 1$. This corresponds to the true Born region. The closer E_1 approaches ω, the larger is the unphysical region, viz., $|\cos\theta_2|>1$ region. When this occurs extrapolation of the experimental GOS through the unphysical region to its value at $K^2=0$ becomes difficult.

Case B. $x_1<\cos\theta_1$:



In this case there is no value of x_2 which would make $|\cos\theta_2| \leq 1$. Hence, when $x_1 = \sqrt{1-\omega/E_1} < \cos\theta_1$, $\cos\theta_2$ is unphysical.

To obtain the desired extrapolation formula, we use the second root of x_2 in Eq. (9), viz., $x_1(x_1 - \cos\theta_1)/(1-x_1\cos\theta_1)$ and rewrite it as

$$-F_{\text{extrap}}(x,y) = \left[1 + \frac{x^2-1}{1-x\cos\theta}\right], \tag{10}$$

where we have replaced x_1 with x. Rather than use $\cos\theta$ as the variable in Eq. (10), let us use y with no restriction to its value. We note that Eq. (10) has the proper behavior, viz., $\lim_{x\to 1} F_{\text{extrap}} \to 1$ and $\lim_{x\to 0} F_{\text{extrap}} \to 0$. The former implies the true Born region ($y=1$), $E\to\infty$, while the latter represents $E\to\omega$, strong non-Born region. Note that (i) from Eq. (2), when $K^2=0$, $y \equiv y_0 = (1+x^2)/2x$ which may be physical $y_0 \leq 1$ or unphysical $y_0 > 1$, and that (ii) Eq. (10) is physically applicable only for small K^2 values.

The proper behavior of Eq. (10) in the limit $x\to 1$ and the slow variation of the dipole matrix elements as $K^2 \to 0$ suggest the use of Eq. (10) in the construction of an extrapolation formula to reach $K^2=0$. At exactly $K^2=0$ we know that by definition $f_{0n}^G(K) = f^0$ and that $F_{\text{extrap}}=1$, regardless of the value of E. Therefore, we can write

$$\begin{aligned}\lim_{K^2\to 0} f_{0n}^G(K) &\equiv f^0 \\ &= \lim_{K^2\to 0}[f^0 F_{\text{extrap}}(x,y)] \\ &= f^0 \lim_{K^2\to 0} F_{\text{extrap}}(x,y) \\ &= -f^0 \lim_{y\to y_0}\left[1+\frac{x^2-1}{1-xy}\right].\end{aligned} \tag{11}$$

In the region of small K^2, we can still write Eq. (11) approximately as

$$f_{0n}^G(K) = -f^0\left[1+\frac{x^2-1}{1-xy}\right]. \tag{12}$$

We must stress that the range of K^2 values for which Eq. (12) is applicable must be determined through comparison with measurements and that its beauty lies in that it can be studied as a function of scattering angle y ($\equiv\cos\theta$) or K^2 for fixed x (impact energy) for a given allowed dipole transition. Clearly, for forward scattering $y=1$ ($\theta=0$) and $E=\infty$, Eq. (12) gives $f_{0n}^G(K)=f^0$, the Lassettre limit theorem. This is the only case for which $K^2=0$ corresponds to physical angles. For any other impact energy value, $K^2=0$ corresponds to unphysical angles so that extrapolation of the GOS through the unphysical region will be necessary to reach the optical oscillator strength. The largest value of K^2 for which Eq. (12) is applicable can only be determined through comparison of the calculated values of $f_{0n}^G(K)$ from Eq. (12) with those obtained from experimental differential cross sections using Eq. (1). Equation (11) can also be used to normalize the experimentally determined relative differential cross sections at any impact energy through Eq. (1).

In using Eq. (12) for normalization of measured small-angle differential cross sections, one selects a value for y in the physical region where the measurements are accurate and obtains $x=\sqrt{1-\omega/E}$, and hence K^2. Then Eqs. (10) and (12) are employed to obtain F_{extrap} and $f_{0n}^G(K)$. Note that normalization will require an energy-dependent normalization factor as was suggested by Msezane and Henry [11]. Conversely, if f^0 is unknown, the ratio $-f_{0n}^G(K)/f^0 \equiv 1+(x^2-1)/(1-xy)$ is obtained for given x and y as well as $f_{0n}^G(K)$ from Eq. (1). Then f^0 can be determined. The accuracy of f^0 thus obtained will depend upon how accurately the differential cross section for optically allowed transitions is measured near $y=1$. Generally, the differential cross section is highly peaked in the forward direction [7,16] so that better accuracy may be obtained away from $\theta=0$. The reason is that measurements are generally difficult and unreliable near $\theta=0$.

III. RESULTS

To demonstrate the validity of the Lassettre limit theorem regardless of impact energy, we show in Table I the variation of $F_{\text{extrap}}(x,y)$ with y and K^2 at $E=20$, 100, and 400 eV for the Xe $5p^6(^1S_0)\to 5p^5(^2P_{3/2})6s$ transition. The function $F_{\text{extrap}}(x,y)$ approaches unity as $K^2\to 0$ independently of E. It is seen from Table I that the smaller the value of E, the greater is the unphysical region [the region between $y=1$ and $y_0=(1+x^2)/2x$, corresponding to $\theta=0$ and $K^2=0$, respectively]. Because of normalization, $F_{\text{extrap}}=1$ at $K^2=0$, regardless of the value of E. Furthermore, the difference between the value of F_{extrap} at $K^2=0$ and $y=1$ measures the amount by which a given transition deviates from the true Born approximation. Consequently, the value of F_{extrap} is unity at $y=1$ ($\theta=0$) for the true Born approximation ($E=\infty$). For clarity, compare the values of F_{extrap} at $y=1$ for $E=20$, 100, and 400 eV; they are 0.767 40, 0.956 89, and 0.989 40, respectively. Depending upon the desired accuracy, one can determine *a priori* whether a given transition can be analyzed through the Born approximation by checking the value of F_{extrap} at $y=1$ ($\theta=0$); it should be unity. Accordingly, the Xe $5p^6(^1S_0)\to 5p^5(^2P_{3/2})6s$ transition at 100 eV is still non-Born while at 400 eV it is almost in the Born region.

In Fig. 1 we have plotted the universal function $F(y) \equiv +F_{\text{extrap}}(x,y)$ versus y for the Xe $5p^6(^1S_0)\to 5p^5(^2P_{3/2})6s$ transition ($\omega=8.436$ eV) for $E=8.5$, 10, 20, 50, 250, and 500 eV. The origin is at $y=1$ ($\theta=0$) and $F(y)=0$ and the family of curves lies almost entirely in the physical region ($y\leq 1$) for $E \gg \omega$ and in both the physical and unphysical ($y>1$) regions for E of the order of ω. The most significant revelation of the plots is that the line $F(y)=1$ corresponds to $K^2=0$ regardless of the value of E. Furthermore, each E curve has associated with it a pole (vertical lines) and a zero at $K^2=0$. The pole and the zero are coincident and are in the physical region only for $E=\infty$, but separate in the unphysical region. Interestingly, the pole moves away from the $y=1$

TABLE I. Values of the universal function, F_{extrap} vs K^2 (a.u.). Values in bold correspond to unphysical values of y.

$E=20$ eV			$E=100$ eV			$E=400$ eV		
y	F_{extrap}	K^2 (a.u.)	y	F_{extrap}	K^2 (a.u.)	y	F_{extrap}	K^2 (a.u.)
1.037 75	**1.000 00**	**0.000 00**	**1.000 97**	**0.999 95**	**0.000 00**	**1.000 23**	**1.000 00**	**0.000 00**
1.035 00	**0.980 36**	**0.006 15**	**1.000 80**	**0.992 27**	**0.002 41**	**1.000 00**	**0.989 40**	**0.001 65**
1.030 00	**0.945 63**	**0.017 33**	**1.000 50**	**0.978 85**	**0.006 63**	0.999 90	0.971 00	0.009 13
1.020 00	**0.879 70**	**0.039 70**	**1.000 10**	**0.961 24**	**0.012 23**	0.999 70	0.935 21	0.020 77
1.010 00	**0.818 09**	**0.062 06**	**1.000 00**	**0.956 89**	**0.013 67**	0.999 30	0.867 39	0.044 05
1.005 00	**0.788 78**	**0.073 25**	0.999 00	0.914 40	0.027 74	0.998 00	0.676 44	0.119 71
1.000 00	**0.767 40**	**0.084 43**	0.998 00	0.873 71	0.041 81	0.997 00	0.554 20	0.177 91
0.999 00	0.754 83	0.086 66	0.996 00	0.797 31	0.069 96	0.996 00	0.448 57	0.236 11
0.995 00	0.732 90	0.095 61	0.995 00	0.761 41	0.084 03	0.992 00	0.138 94	0.468 91
0.990 00	0.706 25	0.106 79	0.992 00	0.661 80	0.126 24	0.990 00	0.028 97	0.585 31
0.980 00	0.655 33	0.129 16	0.990 00	0.154 38	0.154 38			
0.960 00	0.562 10	0.173 89	0.980 00	0.355 25	0.295 10			
0.940 00	0.478 81	0.218 62						
0.900 00	0.336 31	0.308 07						

axis, as y increases to the left, faster than its corresponding zero as E approaches ω; for example, compare the $E=10$ eV and $E=20$ eV poles and their corresponding zeros along the $F(y)=1$ line.

In the figure, there is a small "physical window" bounded by $y=(1,-1)$ and $F(y)=(-1,1)$. In this window $\lim_{E\to\infty}y_0=\lim_{x\to 1}y_0=1$, which corresponds to the region of first Born approximation. We also note that from Eq. (2) $K^2/2\omega=(1-F_{\mathrm{extrap}})/(1+F_{\mathrm{extrap}})$, which reduces to $K^2=2\omega$ when $F_{\mathrm{extrap}}=0$, corresponding physically to excitation with zero kinetic energy. The smaller energy curves have a much larger unphysical region than the higher energy ones, examples of which are the $E=20$ and 50 eV curves. Note that the $E=50$ eV curve intersects the $y=1$ axis at 0.9118 (this value can be compared with 0.9915 for the $E=500$ eV curve) and has a significant unphysical region.

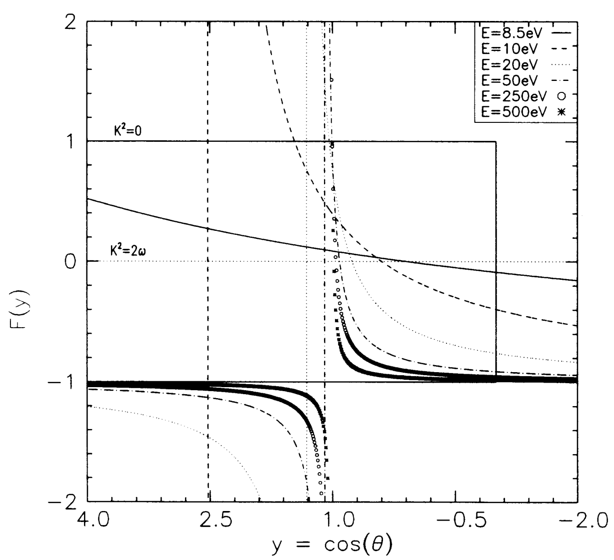


FIG. 1. The universal function $F(y)$ is plotted against y for the Xe $5p^5(^2P_{3/2})6s$ state under the experimental condition of Suzuki *et al.* [7]. Several values of E have been used to demonstrate the physical ($y\le 1$) and unphysical ($y>1$) regions. We note that for each energy curve, $F(y)=+1$ corresponds to $K^2=0$ regardless of the energy. The vertical lines — — —, ..., and —·—·—· correspond to the poles at $K^2=0$, for $E=10$, 20, and 50 eV, respectively.

To test Eq. (12) and determine its range of applicability, we have compared in Fig. 2 our (——) GOS at 300 and 500 eV (the results are the same to the thickness of the line) with the experimental values at 300 eV (●) and 500 eV (▲) by Takayanagi *et al.* [7] for the Kr $4p^6\to 4p^5(^2P_{3/2})5s$ dipole allowed transition. Agreement between the calculated and measured values is very good for $K^2\le 0.1$ a.u.; the interest of this paper is in the region of small K^2. In Fig. 3 the experimental values (▲) of Williams *et al.* [17] are contrasted with the current values (——) at 50 eV for the Mg II $3s\to 3p$ transition. Good agreement is obtained between theory and measurement for $K^2\le 0.1$ a.u. Also are included the theoretical data (— — —) of Msezane and Henry [18].

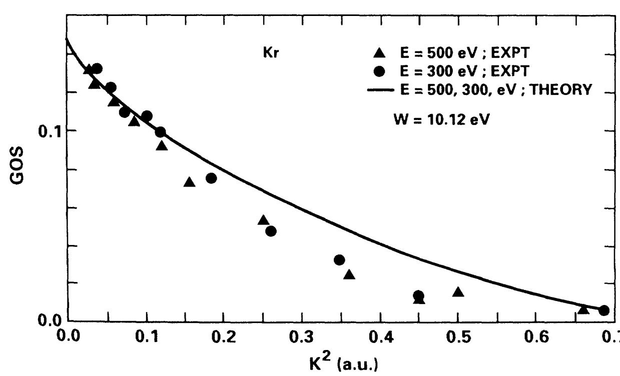


FIG. 2. Generalized oscillator strength (GOS) vs K^2 (a.u.) for the Kr $4p^6\to 4p^5(^2P_{3/2})5s$ transition. The experimental values $E=500$ eV (▲) and $E=300$ eV (●) of Takanayagi *et al.* [7] are compared with the theoretical curve (——) obtained at $E=500$ and 300 eV. To the thickness of the theoretical line the values at $E=500$ and 300 eV are indistinguishable.

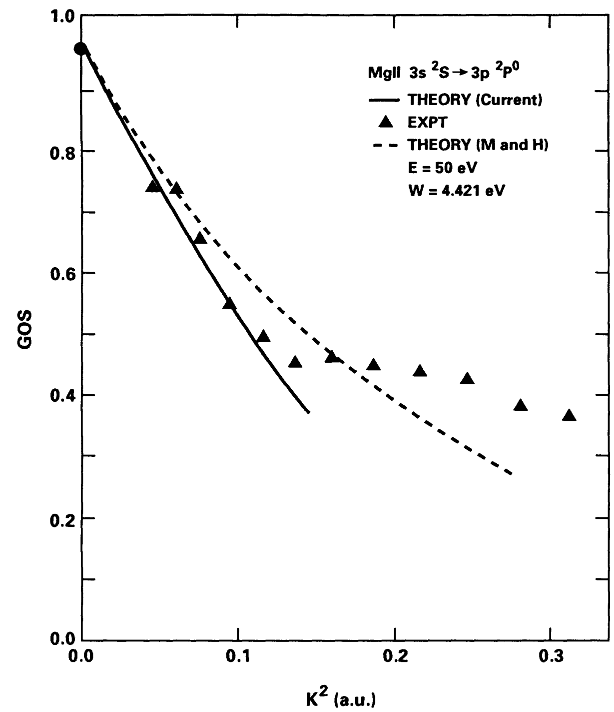


FIG. 3. The GOS from the small-angle differential cross section measurement of Williams *et al.* [17] for the Mg II $3s\,^2S \rightarrow 3p\,^2P^0$ transition is compared with the current theory (——) and the data of Msezane and Henry [18] (— — —) at $E=50$ eV.

IV. DISCUSSION AND CONCLUSION

In this paper, we have derived rigorous bounds on K^2 and used them to construct a universal function F_{extrap} to extrapolate the GOS through the unphysical region to the optical oscillator strength. F_{extrap} has been used to demonstrate unambiguously the validity of the Lassettre limit theorem through the Xe $5p^6 \rightarrow 5p^5(^2P^0_{3/2})6s$ dipole allowed transition regardless of electron-impact energy. Also, the dipole allowed transitions Kr $4p^6 \rightarrow 4p^5(^2P^0_{3/2})5s$ at 500 and 300 eV and Mg II $3s \rightarrow 3p$ at 50 eV have been used to determine the range of applicability of F_{extrap} through comparison of the GOS values obtained from it with those obtained from the measured small-angle differential cross sections. The soundness of our extrapolation function is further supported by the most recent calculation by Mitroy [19] for the K $4s \rightarrow 4p$ transition at 54.4 and 100 eV. At both energies there is excellent agreement between our data and Mitroy's UDWBA results given in his Figs. 3(a) and 4(a) (we do not show the results), including the measurements [20,21], particularly the data of Vuskovic and Srivastava [20] for $K^2 \leq 0.05$ a.u. This comparison demonstrates that the GOS for the K $4s \rightarrow 4p$ transition is almost the same at 54.4 and 60 eV in the limit $K^2 \rightarrow 0$, viz., away from the diffraction minima of the differential cross section.

We conclude that our universal extrapolation function produces results that are in excellent agreement with measurements and other theory for $K^2 \leq 0.05$ a.u. (conservatively). The ultimate test of a theory is its ability to produce results that are compatible with measurements. Further theoretical justification of our derivation is found in the assumption of the pole dominance of the single photon exchange in the K^2 crossed channel embedded in the Lassettre limit theorem. It leads to the proportionality of the optical oscillator strength to the residue of the differential cross section at $K^2=0$ [22]. Clearly, in the limit $K^2 \rightarrow 0$ kinematical considerations are the main determinants of the behavior of the GOS. We note that high energy and small K^2 require equivalent theoretical approximations. It is therefore not surprising that the Lassettre limit theorem is valid in the Born approximation as well as at small K^2 values. The advantage of our extrapolation function is its rigor and simplicity, having been derived from rigorous bounds on K^2. F_{extrap} is by no means the only possible extrapolation function that can be constructed from the bounds on K^2. For example, another function $X_{\text{extrap}}(K^2) = -[1-2/(1+K^2/2w)^y]$ is possible, where y varies from 0.2 through 5.0 and we have used Eq. (2) and the value of x to eliminate x^2 and $x\cos\theta$ in Eq. (10). When $y=1.0$, we recover Eq. (10). The function $X_{\text{extrap}}(K^2)$ can increase/decrease the range of applicability of Eq. (12) depending upon the value of y used. The expression for $X_{\text{extrap}}(K^2)$ is only a function of K^2 for a given transition, thus demonstrating the validity of the Lassettre limit theorem, regardless of the impact energy.

We have focused our investigation to the region of small K^2 values because this region is difficult to access both experimentally and theoretically, particularly for moderate and small impact energies. Obviously, dynamical effects will become important as K^2 increases from zero. How to include these effects for larger K^2 values will be the subject of our future investigation. Suffice it to say that our current interest has been in the region of small scattering angles where most experimental uncertainties occur.

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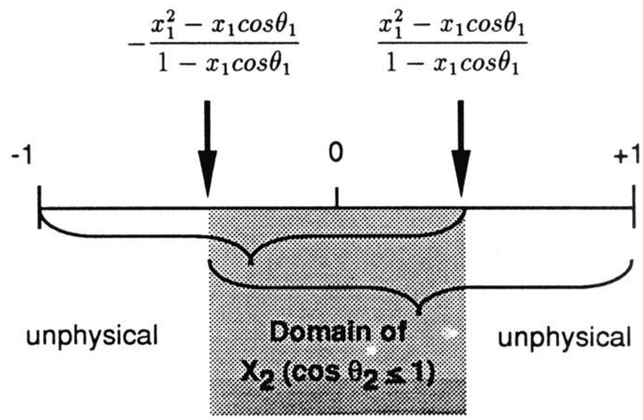
$-\frac{x_1^2 - x_1 cos\theta_1}{1 - x_1 cos\theta_1}$
$\frac{x_1^2 - x_1 cos\theta_1}{1 - x_1 cos\theta_1}$
-1
0
+1
unphysical
Domain of
X_2 ($\cos\theta_2 \leq 1$)
unphysical