Formula for the calculation of integral cross sections in a Fourier expansion method

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A method has been developed to calculate the integral cross sections from the measured generalized oscillator strengths that are fitted by a Fourier expansion. The method has been applied to the e-Xe and e-N$_2$ scattering problems. Excellent agreement has been obtained with existing measured values for the transitions to $5p^5(^2P_{3/2})6s$ and $5p^5(^2P_{1/2})6s$ of Xe at 100 and 500 eV. For the vibrational states, $v=1$–4, of the $b^1\Pi_u$ electronic state of N$_2$ at 300 eV, good agreement with the data calculated by the Lassettre expansion has also been achieved. [S1050-2947(97)09501-2]

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One of the main purposes in the measurement of differential cross sections (DCS's) is to obtain integral cross sections (ICS's). Since DCS's for optically allowed transitions increase dramatically as the scattering angle decreases, experimentalists begin their measurement at a small angle θ_m to avoid the region where the measurements are likely to have large uncertainties. However, DCS's at scattering angles less than θ_m usually contribute significantly to ICS's, particularly when the impact energies are high [1]. In order to obtain reliable ICS's, researchers normally transform DCS's into generalized oscillator strengths (GOS's) and integrate them with respect to the momentum transfer squared, K^2 [2],

$$\sigma = \frac{\pi}{Ew} \int_{K^2_{\min}}^{K^2_{\max}} f(K^2) \frac{dK^2}{K^2}, \qquad (1)$$

where E is the impact energy, w is the excitation energy, and $f(K^2)$ is the GOS function. In the evaluation of Eq. (1) the Lassettre expansion [3] has been used widely to fit the GOS data, because it has the correct singularity for the scattering amplitude and is able to fit all the values of K^2. The Lassettre series for the s-p transition has the form

$$f(K^2) = \frac{f_0}{(1+x)^6} \left[1 + f_1\left(\frac{x}{1+x}\right) + f_2\left(\frac{x}{1+x}\right)^2 + \cdots \right], \qquad (2)$$

where f_0 is the optical oscillator strength (OOS), $x=K^2/\alpha^2$, and $\alpha=\sqrt{2I}+\sqrt{2(I-w)}$, with I being the ionization energy and w the excitation energy. The coefficients $f_0, f_1, f_2 \ldots$ are determined by the least-square calculation. Substituting Eq. (2) into Eq. (1) we obtain the expression for calculating ICS's [4],

$$\sigma = \frac{\pi}{Ew} [\ln(8cE) - \phi] f_0, \qquad (3)$$

where c and ϕ are calculated from the equations

$$\ln c = 2\ln\left(\frac{\alpha}{2w}\right) - \frac{137}{60} + \frac{f_1}{6} + \frac{f_2}{42} + \frac{f_3}{168} + \frac{f_4}{504} + \frac{f_5}{1260} \qquad (4)$$

and

$$\phi = \frac{w}{2E} + \frac{(f_1-6)w^2}{2\alpha^2 E}, \qquad (5)$$

with $f_1, f_2, f_3 \ldots$ being the coefficients of $[(x/(1+x)]^n$, $n=1,2,3 \ldots$.

Equation (2) has also been used by experimentalists to extrapolate GOS's to $K^2=0$ to obtain OOS's. However, as Eq. (2) is an infinite series the OOS obtained is dependent on the number of terms retained. Recently, Haffad *et al.* [5] used a Fourier expansion to fit GOS's, with the function $f(K^2)$ expressed as

$$f(K^2) = \frac{1}{(1+x)^6} [a_0 + a_1\cos(\epsilon y) + b_1\sin(\epsilon y)], \qquad (6)$$

where $y=\ln(1+x)$, and x has the same meaning as in Eq. (2). The coefficients a_0, a_1, b_1, and ϵ are determined by least-square calculation. Substituting Eq. (6) into Eq. (1), we have

$$\sigma = \frac{\pi}{Ew} \int_{K^2_{\min}}^{K^2_{\max}} \frac{1}{(1+x)^6}$$
$$\times [a_0 + a_1\cos(\epsilon y) + b_1\sin(\epsilon y)] \frac{dK^2}{K^2}. \qquad (7)$$

Equation (7) cannot be evaluated directly. However, it can be transformed into

TABLE I. Coefficients of Eq. (6) for the transitions to $5p^5(^2P_{1/2})6s$ and $5p^5(^2P_{3/2})6s$ of Xe. The numbers in the brackets of Tables I, II, and IV are the power of 10 by which the coefficients should be multiplied.

	100 eV		500 eV	
	$^2P_{1/2}$	$^2P_{3/2}$	$^2P_{1/2}$	$^2P_{3/2}$
a_0	0.3638	0.1795	0.4308	0.2950
a_1	−0.1940	0.3552(−1)	−0.2544	−0.7927(−1)
b_1	−0.2645	−0.1438	−0.3199	−0.2629
ϵ	3.600	0.7229(+1)	0.3136(+1)	0.4498(+1)

TABLE II. Coefficients of Eq. (6) for the transitions to the vibrational states, $v=1–4$, of the $b^1\Pi_u$ electronic state of N_2.

	$v=1$	$v=2$	$v=3$	$v=4$
a_0	0.142 716 85(−1)	−0.165 834 38(+3)	−0.157 899 19(+3)	0.127 799 80(+4)
a_1	−0.128 815 06(−3)	0.165 858 18(+3)	0.157 941 95(+3)	−0.127 791 55(+4)
b_1	−0.178 562 27(−2)	0.136 044 07(+1)	−0.145 881 74(+1)	−0.796 048 27(+1)
ϵ	0.270 374 89(+2)	0.626 991 57(−1)	−0.887 365 82(−1)	0.354 848 16(−1)

$$\sigma = \frac{\pi}{Ew} \int_{x_{\min}}^{x_{\max}} \frac{1}{x(1+x)^6} \left[a_0 + \left(\frac{a_1}{2} + \frac{b_1}{2i} \right)(1+x)^{i\epsilon} \right.$$
$$\left. + \left(\frac{a_1}{2} - \frac{b_1}{2i} \right)[(1+x)^{-i\epsilon}] \right] dx, \qquad (8)$$

where $x_{\min} = K_{\min}^2/\alpha^2$ and $x_{\max} = K_{\max}^2/\alpha^2$. To evaluate Eq. (8) the integrand has to be expanded over the whole complex plane. We construct a loop in the complex plane using two lines, $x_{\min} + iy(y=0 \to \infty)$ and $x_{\max} + iy(y=\infty \to 0)$, part of the real axis $x_{\min}$ to $x_{\max}$ and the line $x_{\min} + i\infty$ to $x_{\max} + i\infty$. As $x_{\min}$ and $x_{\max}$ are greater than zero, there is no singularity inside the loop. Also, the contribution to the integral from the final part of the loop can be ignored as $y \to \infty$ the integrand $\to 0$. The original integration from $x_{\min}$ to $x_{\max}$ then reduces to the integral from 0 to ∞ along the line $x=x_{\min}$ plus ∞ to 0 on the line $x=x_{\max}$. The integration of Eq. (8) is carried out in the Appendix.

With the values of I_I, I_{II}, and I_{III} from the Appendix, Eq. (8) reduces to

$$\sigma = \frac{\pi}{Ew} \left[a_0 I_{III} + \left(\frac{a_1}{2} + \frac{b_1}{2i} \right) I_I + \left(\frac{a_1}{2} - \frac{b_1}{2i} \right) I_{II} \right]. \qquad (9)$$

Since the cross section is a real number, the integrals I_I and I_{II} must be the complex conjugate of each other. In the calculation of σ we only need to evaluate the integral I_I or I_{II}. Let us consider a hypergeometric function $_2F_1(a,b;c;z)$, with $b=1$ and $c=1+a$. This kind of a hypergeometric function can be expressed as

$$_2F_1(a,b;c;z) = a \sum_{n=0}^{n=\infty} \frac{z^n}{a+n}. \qquad (10)$$

In the case of $z=1/(1+x_{\max})$ the convergence can usually be obtained by keeping only a few terms in the expansion. The β function in the I_I and I_{II} of Eq. (9) can be found in many mathematical libraries.

Equation (9) was used to calculate the excitation cross section for the e-Xe and e-N_2 scattering. The GOS data are taken from the measurements of Suzuki $et\ al.$ [2] for Xe and Xu $et\ al.$ [6] for N_2. The coefficients in Eq. (6) for the transitions to the $5p^5(^2P_{3/2})6s$ and $5p^5(^2P_{1/2})6s$ states of Xe are listed in Table I, while those of the vibrational states, $v=1–4$, of the $b^1\Pi_u$ electronic state of N_2 are given in Table

II. For vibrational states 3 and 4, the coefficients a_0 and a_1 are close to each other. Therefore, we keep eight significant digits to achieve high accuracy. Table III gives ICS's for the e-Xe scattering using Eqs. (3) and (9). The Suzuki $et\ al.$ data which was obtained by fitting GOS's with the Lassettre equation and performing a numerical calculation, are also listed in Table III. An excellent agreement among the three sets of data has been achieved. This demonstrates that the data are well described by Eq. (6), as can be see in the paper by Haffad $et\ al.$ [5]. Table IV presents the coefficients of Eq. (2) for the e-N_2 collision. If we retain more than four terms in the Lassettre expansion, the curve fits are more noisy. Therefore, only four terms have been used in the fitting.

In Table V, ICS's calculated using Eq. (9) are compared with those from Eq. (3). The agreement between the results of the two methods is satisfactory. We note that the fitting process and fitting function are quite different in the two methods. However, the difference between the OOS's obtained by the two methods is small. This is probably the reason why the ICS's obtained by the two methods agree with each other so well, as well as the fact that at high energy most of the contribution to the integral cross section comes from small scattering angles, or small K^2 values. In this region of small-K^2 values the GOS's are close to the OOS's.

In conclusion, a formula has been obtained to calculate the integral cross sections when the GOS's are fitted by a Fourier series. The formula was illustrated through a calculation of ICS's for the e-Xe and the e-N_2 collision problems. Good agreement was achieved when the results are compared with those from other methods.

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TABLE III. ICS's (10^{-16} cm^2) for the e-Xe scattering.

	100 eV		500 eV	
	$^2P_{1/2}$	$^2P_{3/2}$	$^2P_{1/2}$	$^2P_{3/2}$
Eq. (3)	0.2083	0.3565	0.073 94	0.1236
Eq. (9)	0.2080	0.3560	0.079 89	0.1230
Suzuki	0.204	0.352	0.0751	0.126

TABLE IV. Coefficients of Eq. (2) for the transitions to the vibrational states $v=1$–4 of the $b^1\Pi_u$ electronic state of N_2.

	$v=1$	$v=2$	$v=3$	$v=4$
f_0	0.1441(−1)	0.3173(−1)	0.5108(−1)	0.8124(−1)
f_1	−0.6001(+1)	−0.6218(+1)	−0.3099(+1)	−0.3272(+1)
f_2	0.8515(+2)	0.7346(+2)	0.3966(+2)	0.9403(+1)
f_3	−0.2733(+3)	−0.2272(+3)	−0.1428(+3)	0.7920

APPENDIX: INTEGRATION OF EQ. (8)

The integration $\int_{x_{min}}^{x_{max}}(dx/[x(1+x)^{6-i\epsilon}])$ can be separated into two parts:

$$I_I = \int_{x_{min}}^{x_{max}} \frac{dx}{x(1+x)^{6-i\epsilon}}$$

$$= \int_0^\infty \frac{1}{(1+x_{min}+iy)^{6-i\epsilon}} \frac{i}{(x_{min}+iy)} \, dy$$

$$- \int_0^\infty \frac{1}{(1+x_{max}+iy)^{6-i\epsilon}} \frac{i}{x_{max}+iy} \, dy. \quad \text{(A1)}$$

Integral I_I can be evaluated to obtain

$$I_I = B(1,6-i\epsilon)\left[\frac{{}_2F_1\left(6-i\epsilon,1;7-i\epsilon; \frac{1}{1+x_{min}}\right)}{(1+x_{min})^{6-i\epsilon}} \right.$$

$$\left. - \frac{{}_2F_1\left(6-i\epsilon,1;7-i\epsilon; \frac{1}{1+x_{max}}\right)}{(1+x_{max})^{6-i\epsilon}} \right]. \quad \text{(A2)}$$

A similar formula can be obtained for integral I_{II}:

TABLE V. ICS's (10^{-17} cm^2) for the transitions to the vibrational level $v=1$–4 of the $b^1\Pi_u$ electronic state of N_2.

	$v=1$	$v=2$	$v=3$	$v=4$
Eq. (9)	0.075 14	0.1297	0.2317	0.4783
Eq. (3)	0.065 82	0.1406	0.2407	0.3919

$$I_{II} = \int_{x_{min}}^{x_{max}} \frac{dx}{x(1+x)^{6+i\epsilon}}$$

$$= B(1,6+i\epsilon)\left[\frac{{}_2F_1\left(6+i\epsilon,1;7+i\epsilon; \frac{1}{1+x_{min}}\right)}{(1+x_{min})^{6+i\epsilon}} \right.$$

$$\left. - \frac{{}_2F_1\left(6+i\epsilon,1;7+i\epsilon; \frac{1}{1+x_{max}}\right)}{(1+x_{max})^{6+i\epsilon}} \right]. \quad \text{(A3)}$$

The third integral is

$$I_{III} = \int_{x_{min}}^{x_{max}} \frac{dx}{x(1+x)^6}$$

$$= \frac{1}{5(1+x_{max})^5} + \frac{1}{4(1+x_{max})^4} + \frac{1}{3(1+x_{max})^3}$$

$$+ \frac{1}{2(1+x_{max})^2} + \frac{1}{(1+x_{max})} - \frac{1}{5(1+x_{min})^5}$$

$$- \frac{1}{4(1+x_{min})^4} - \frac{1}{3(1+x_{min})^3} - \frac{1}{2(1+x_{min})^2}$$

$$- \frac{1}{(1+x_{min})} + \ln\left(\frac{x_{max}}{1+x_{max}}\right) - \ln\left(\frac{x_{min}}{1+x_{min}}\right). \quad \text{(A4)}$$

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