Analytical expression for higher-order derivatives of the Lewis integral with its application to proton–hydrogen charge transfer collisions

Utpal Roy and N C Sil

Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta-700032, India

Abstract. We present a method for evaluating arbitrary higher-order derivatives of the three-denominator Lewis integral frequently encountered in collisional and structural problems of atomic and molecular physics. The method has been applied successfully to obtain analytical expressions for the $ns \to n's$ charge transfer amplitude in proton–hydrogen collisions and the results for total cross sections in Jackson–Schiff (JS) and distorted-wave approximations (DWB) are presented.

1. Introduction

During an application of the second Born approximation to the scattering of high-energy electrons from a model potential representing a rather generalized charge distribution of the atomic nuclei, Lewis was led to consider the problem of evaluation of the integral [1] (hereafter denoted by $\mathcal{L}$)

$$\mathcal{L}(\lambda; \boldsymbol{q}_1, \mu_1; \boldsymbol{q}_2, \mu_2) = \int \frac{\mathrm{d}\boldsymbol{q}}{(q^2 + \lambda^2)(|\boldsymbol{q} - \boldsymbol{q}_1|^2 + \mu_1^2)(|\boldsymbol{q} - \boldsymbol{q}_2|^2 + \mu_2^2)}. \tag{1}$$

He obtained an elegant expression of the integral in the closed form

$$\mathcal{L} = \pi^2 \frac{1}{\mathrm{i}N^{1/2}} \log \frac{\beta + \mathrm{i}N^{1/2}}{\beta - \mathrm{i}N^{1/2}} \tag{2}$$

where

$$N = \alpha\gamma - \beta^2 \tag{3}$$

$$\alpha\gamma = \left[|\boldsymbol{q}_1 - \boldsymbol{q}_2|^2 + (\mu_1 + \mu_2)^2 \right] \left[q_1^2 + (\mu_1 + \lambda)^2 \right] \left[q_2^2 + (\mu_2 + \lambda)^2 \right] \tag{4}$$

and

$$\beta = \lambda \left[|\boldsymbol{q}_1 - \boldsymbol{q}_2|^2 + (\mu_1 + \mu_2)^2 \right] + \mu_2 \left[\lambda^2 + q_1^2 + \mu_1^2 \right] + \mu_1 \left[\lambda^2 + q_2^2 + \mu_2^2 \right]. \tag{5}$$

Evidently the Lewis function $\mathcal{L}$ is single-valued even when one crosses the branch cut of $N^{1/2}$ and it is analytic for complex values λ, μ_1 and μ_2; the arguments of the numerator and denominator of the log function should be taken to lie between $-\pi$ and $+\pi$.

The Lewis function is singular only when $\alpha\gamma = 0$. It can be shown that for real positive values of λ, μ_1 and μ_2, the expression $N = (\alpha\gamma - \beta^2)$ is positive definite for nonzero values

of q_1 and q_2 and it is exactly zero when $q_1 = q_2 = 0$. For such cases it is convenient to write equation (2) as

$$\mathcal{L} = \frac{2\pi^2\theta}{N^{1/2}} \tag{6}$$

with

$$\theta = \tan^{-1}\left(\frac{N^{1/2}}{\beta}\right). \tag{7}$$

Sil and co-workers have used this result widely in the studies of charge transfer in ion–atom collisions, excitation and ionization in electron–atom and positron–atom collisions, positronium formation in positron–atom collisions, etc [2–10]. In general, one requires the evaluation of the Lewis integral together with its various multi-order derivatives with respect to the parameters in order to reduce the matrix elements to closed analytic forms in particle–atom, particle–molecule, particle–nuclei, photon–atom/molecule collisions [11–13]. However, when multi-order derivatives of this integral are present, it is rather difficult to obtain the result analytically.

Recently, by making use of the contour integration technique, Roy *et al* [9] presented a method of evaluation of the multi-order derivatives of the Lewis integral. The results were expressed in terms of two elementary terminating series which are exactly amenable to numerical computation. Although the final expressions possess a large degree of symmetry that can be useful in obtaining higher-order derivatives, attempts to evaluate derivatives of order higher than three had no success.

In this paper, we present a more powerful alternative method of evaluation of the multi-order derivatives of $\mathcal{L}$. Using β and N as the variables, we are able to obtain derivatives of arbitrary higher orders of the Lewis integral with respect to the parameters λ, μ_1 and μ_2 in a closed analytic form. It is pertinent to mention here that, while investigating the Born–Oppenheimer amplitude for transition from an arbitrary initial state to an arbitrary final state $nlm \rightarrow n'l'm'$, Deb and Sil [10] have obtained another closed-form expression for the higher-order derivatives of the integral (1) for the special case $\lambda = 0$. Some low-order derivatives of this special type of Lewis integral have also been evaluated as one-dimensional integrals earlier in the calculation of charge-transfer amplitudes by Bates and Dalgarno [16], and Jackson and Schiff [17]. As a check of our results, we have considered $ns \rightarrow n's$ transitions in the JS and DWB approximations and have compared the computed values with those available in the literature.

Among other analytical works in this direction we mention the interesting investigation of Belkić [18], who evaluated the extended Dalitz integral containing one hydrogenic wavefunction in momentum space together with the Feynman-type two-denominator term. By a suitable choice of the values of the parameters and after an appropriate parametric differentiation one could derive from Belkić's result the 1s–nlm proton–hydrogen charge transfer amplitude in JS and DWB approximations. His result for the extended Dalitz integral was obtained in closed form in terms of seven-variable Lauricella hypergeometric functions. For the convenience of numerical evaluation Belkić suggested expressing such a function, by a suitable transformation to a new set of seven variables, as polynomials in six of these variables, in the remaining variable, however, the function would be an infinite series and so the evaluation problem would still remain.

This paper is structured as follows. In section 2, we describe in detail our analytical formulation for obtaining the higher-order derivatives of the Lewis integral and in section 3 the applications of the resulting closed-form expressions to charge-transfer processes in proton–hydrogen collisions are discussed. Finally, we make our concluding remarks in

section 4. Atomic units are used in our calculation in which $a_0 = m = e = \hbar = 1$, 1 (au) of energy $(= e^2/a_0) = 27.2$ eV.

2. General structure

The expression for all order derivatives of the Lewis integral with respect to its parameters λ, μ_1 and μ_2 has been obtained from a generalization of the result given in Gradshteyn and Ryzhik [15]. Denoting the Lewis integral $\mathcal{L}$ as $\mathcal{L}(X(\lambda, \mu_1, \mu_2), Z(\lambda, \mu_1, \mu_2))$ with the variables $X = \beta, Z = N$, dependent on the parameters λ, μ_1 and μ_2, we obtain

$$\left(\frac{\partial}{\partial\lambda}\right)^{N_1} \left(\frac{\partial}{\partial\mu_1}\right)^{N_2} \left(\frac{\partial}{\partial\mu_2}\right)^{N_3} \mathcal{L}\left(X(\lambda, \mu_1, \mu_2), Z(\lambda, \mu_1, \mu_2)\right)$$

$$= N_1! N_2! N_3! \sum \frac{\Pi(X_{(\sigma_1\sigma_2\sigma_3)}/\sigma_1!\sigma_2!\sigma_2!)^{r_{\sigma_1\sigma_2\sigma_3}} (Z_{(\nu_1\nu_2\nu_3)}/\nu_1!\nu_2!\nu_3!)^{s_{\nu_1\nu_2\nu_3}}}{\Pi r_{\sigma_1\sigma_2\sigma_3}! s_{\nu_1\nu_2\nu_3}!}$$

$$\times \mathcal{L}_{mn}(X, Z) \tag{8}$$

where $\sum$ denotes summation over all solutions in non-negative integers of the following equations:

$$\sum r_{\sigma_1\sigma_2\sigma_3} = m \tag{9}$$

$$\sum s_{\nu_1\nu_2\nu_3} = n \tag{10}$$

$$\sum \sigma_1 r_{\sigma_1\sigma_2\sigma_3} + \sum \nu_1 s_{\nu_1\nu_2\nu_3} = N_1 \tag{11}$$

$$\sum \sigma_2 r_{\sigma_1\sigma_2\sigma_3} + \sum \nu_2 s_{\nu_1\nu_2\nu_3} = N_2 \tag{12}$$

$$\sum \sigma_3 r_{\sigma_1\sigma_2\sigma_3} + \sum \nu_3 s_{\nu_1\nu_2\nu_3} = N_3 \tag{13}$$

and

$$\mathcal{L}_{mn}(X, Z) = \frac{\partial^m}{\partial X^m} \frac{\partial^n}{\partial Z^n} \mathcal{L}(X, Z) \tag{14}$$

$$X_{(\sigma_1\sigma_2\sigma_3)} = \left(\frac{\partial}{\partial\lambda}\right)^{\sigma_1} \left(\frac{\partial}{\partial\mu_1}\right)^{\sigma_2} \left(\frac{\partial}{\partial\mu_2}\right)^{\sigma_3} X(\lambda, \mu_1, \mu_2) \tag{15}$$

$$Z_{(\nu_1\nu_2\nu_3)} = \left(\frac{\partial}{\partial\lambda}\right)^{\nu_1} \left(\frac{\partial}{\partial\mu_1}\right)^{\nu_2} \left(\frac{\partial}{\partial\mu_2}\right)^{\nu_3} Z(\lambda, \mu_1, \mu_2). \tag{16}$$

2.1. Evaluation of $\mathcal{L}_{mn}$

We shall evaluate $\mathcal{L}_{mn}$ in two steps: (i) for nonzero values of m and (ii) for zero values of m. For nonzero values of m we have from equations (6) and (7)

$$\frac{\partial\mathcal{L}}{\partial X} = -\frac{2\pi^2}{(X^2 + Z)}. \tag{17}$$

Thus the expression of $\mathcal{L}_{mn}$ is obtained as

$$\mathcal{L}_{mn}(X, Z) = (-1)^{m+n} 2\pi^2 n! \left(-\frac{\partial}{\partial X}\right)^{m-1} \frac{1}{(X^2 + Z)^{n+1}}. \tag{18}$$

To evaluate the derivative with respect to X in the above expression, we use the formula

$$\left(-\frac{\partial}{\partial\lambda}\right)^n = \sum_{k=0}^{[n/2]} \frac{(-1)^n (2\lambda)^{n-2k} n!}{(n-2k)! k!} \left(\frac{\partial}{\partial\lambda^2}\right)^{n-k} \tag{19}$$

where $[n/2]$ is the nearest integer less than or equal to $n/2$. Finally, the expression for $\mathcal{L}_{mn}$ is reduced to the form

$$\mathcal{L}_{mn}(X, Z) = \frac{2^m \pi^2 X^{m-1}(m+n-1)!}{(X^2+Z)^{m+n}}(-1)^{n+m}$$
$$\times {}_2F_1\left(-\frac{m-1}{2}, -\frac{m-2}{2}; n+m-1; \frac{(X^2+Z)}{X}\right). \tag{20}$$

To evaluate the expression for $\mathcal{L}_{mn}(X, Z)$ when $m = 0$, we make use of the integral representation

$$\mathcal{L} = 2\pi^2 \int_X^\infty \frac{dx}{(x^2+Z)} \tag{21}$$

which can be easily verified. Now

$$\frac{\partial^n \mathcal{L}}{\partial Z^n} = (-1)^n 2\pi^2 n! \frac{1}{N^{n+1/2}} \int_{\phi_0}^{\pi/2} \cos^{2n}\phi \, d\phi \tag{22}$$

where $\phi_0 = \tan^{-1}(X/N^{1/2})$. Ultimately the expression for $\mathcal{L}_{0N}$ is reduced to the form

$$\mathcal{L}_{0n} = \frac{\partial^n \mathcal{L}}{\partial N^n} = (-1)^n n! \frac{2\pi^2}{N^{n+1/2}}\left[\frac{1}{2^{2n}}\binom{2n}{n}\theta + \frac{1}{2^{2n-1}}\sum_{k=0}^{n-1}(-1)^{n-k}\binom{2n}{k}\frac{\sin 2(n-k)\theta}{2(n-k)}\right]. \tag{23}$$

It is interesting to note here the fact that with the present choice of the variable $Z(= \alpha\gamma - \beta^2)$ we have a method which is much simpler and more elegant for generating $\mathcal{L}_{mn}$, the derivatives of $\mathcal{L}$ with respect to X and Z. To arrive at the final expression, we now require the various derivatives of $X(= \beta)$ and $Z(= N)$ with respect to λ, μ_1 and μ_2, which are finite in number and can be easily calculated. We have developed a computer code to evaluate the expression for arbitrary order derivatives of the Lewis integral.

3. Application: proton–hydrogen charge-transfer collision

As an illustration of a physical process that gives rise to the class of integrals, discussed in the earlier sections, we examine the evaluation of the $ns \to n's$ transition amplitude for charge transfer in proton–hydrogen scattering in the Jackson–Schiff (JS) approximation [17]. The first Born amplitude with post-interaction in the Brinkman–Kramers (BK) [19] approximation is

$$I_{BK} = \left(-\frac{\mu_f}{2\pi}\right)\int \Psi_f^*(r_P, R_P)\left(-\frac{Z_T}{r_T}\right)\Psi_i(r_T, R_T)\,dr_T\,dr_P \tag{24}$$

and that in the JS approximation is

$$I_{JS} = \left(-\frac{\mu_f}{2\pi}\right)\int \Psi_f^*(r_P, R_P)V_f\Psi_i(r_T, R_T)\,dr_T\,dr_P \tag{25}$$

with $V_f = (Z_T Z_P/|r_T - r_P| - Z_T/r_T)$, where Z_T and Z_P are the target and projectile charges, respectively. It should be noted that the BK approximation (equation (24)) does not satisfy the correct boundary condition which requires that the perturbing potential is not to exhibit any long-range Coulomb behaviour at large internuclear separations [20, 21]. Though the JS approximation (equation (25)) is, in general, incompatible with this asymptotic requirement it is all right, however, for our proton–hydrogen charge transfer problem with $Z_T = Z_P = 1$.

The initial and final channel wavefunctions $\Psi_i(r_P, R_P)$ and $\Psi_f(r_T, R_T)$ are described by

$$\Psi_f(r_P, R_P) = \exp(iK_f \cdot R_P)\phi_f(r_P) \tag{26}$$

$$\Psi_i(r_T, R_T) = \exp(iK_i \cdot R_T)\phi_i(r_T) \tag{27}$$

where r_T, r_P are, respectively, the position vectors of the electron with respect to the target (T) and the projectile (P) nuclei and R_T, R_P describe the position vector of P with respect to the centre of mass of the initial subsystem (e + T) and the position vector of the centre of mass of the final subsystem (e + P) with respect to T. These Jacobi coordinates are inter-related by

$$r_T = R_P + \beta_1 r_P \qquad r_P = -R_T + \alpha_1 r_T$$

$$R_T = \alpha_1 R_P - (1 - \alpha_1\beta_1)r_p \qquad R_P = \beta_1 R_T + (1 - \alpha_1\beta_1)r_T$$

with $\alpha_1 = M_T/(m + M_T)$ and $\beta_1 = M_P/(m + M_P)$ and $\phi_i(r_T)$ and $\phi_f(r_P)$ are the initial and final bound state wavefunctions of hydrogen with eigenenergies ε_i and ε_f. The conservation of energy gives

$$E = \frac{1}{2\mu_i}K_i^2 + \varepsilon_i = \frac{1}{2\mu_f}K_f^2 + \varepsilon_f \tag{28}$$

where μ_i and μ_f are the three-body reduced masses in the initial and final channels. The BK amplitude can be obtained analytically (cf [2])

$$I_{BK} = \left(-\frac{\mu_f}{2\pi}\right)\frac{32Z_T C_1 C_2 \pi^2 n'}{\gamma_n^2 \gamma_{n'}^3}\frac{1}{pq(q^2+1)}\sin 2n\theta_1 \sin 2n'\theta_2 \tag{29}$$

with

$$p = \frac{J}{\gamma_n} \qquad q = \frac{K}{\gamma_{n'}}$$

$$\theta_1 = \tan^{-1}\frac{1}{p} \qquad \text{and} \qquad \theta_2 = \tan^{-1}\frac{1}{q}.$$

Here

$$K = \beta_1 K_f - K_i \qquad J = \alpha_1 K_i - K_f$$

$$C_1 = \frac{\gamma_n}{2n}\sqrt{\frac{\gamma_n}{\pi}} \qquad C_2 = \frac{\gamma_{n'}}{2n'},\sqrt{\frac{\gamma_{n'}}{\pi}}$$

$$\gamma_n = \frac{\mu Z_T}{n} \qquad \text{and} \qquad \gamma_{n'} = \frac{\mu' Z_P}{n'}$$

where μ and μ' are the two-body reduced masses of initial and final subsystems. With contour representation of the wavefunctions $\phi_i(r_T)$ and $\phi_f(r_P)$ and using the results of the previous sections, one readily obtains the contribution (to the amplitude) due to the inter-nuclear interaction parts only in terms of derivatives of the Lewis integral, i.e.

$$\mathcal{I}_N = \left(-\frac{\mu_f}{2\pi}\right)Z_T Z_P C_1 C_2\left[-8nn'\sum_{r=0}^{n-1}\sum_{r'=0}^{n'-1}\binom{n-1}{r}\binom{n'-1}{r'}\frac{2^{r+r'+2}}{(r+1)!(r'+1)!}\gamma_n^r\gamma_{n'}^{r'}\right.$$

$$\left.\times\mathcal{L}_{(0\,r+1\,r'+1)}(0; -J, \gamma_n; K, \gamma_{n'})\right]. \tag{30}$$

The amplitude in the JS approximation is given by

$$I_{JS} = I_{BK} + \mathcal{I}_N. \tag{31}$$

In the DWB approximation the effective potential is given by [22, 23]

$$V_d = -\frac{Z_T}{r_T} + \frac{Z_T}{|r_T - r_P|} - Z_T \left(Z_P + \frac{1}{|r_T - r_P|} \right) \exp(-2Z_P|r_T - r_P|). \tag{32}$$

For the problem under consideration $Z_T = Z_P = 1$, so one can write down the amplitude for the DWB approximation in exactly the same way

$$I_{DWB} = I_{JS} + \mathcal{I}_{DS}. \tag{33}$$

where

$$\mathcal{I}_{DS} = \left(-\frac{\mu_f}{2\pi} \right) C_1 C_2 8nn' \sum_{r=0}^{n-1} \sum_{r'=0}^{n'-1} \binom{n-1}{r} \binom{n'-1}{r'} \frac{2^{r+r'+2}}{(r+1)!(r'+1)!} \gamma_n^r \gamma_{n'}^{r'}$$
$$\times \left[\mathcal{L}_{(0\,r+1\,r'+1)}(2; -J, \gamma_n; K, \gamma_{n'}) - \mathcal{L}_{(1\,r+1\,r'+1)}(2; -J, \gamma_n; K, \gamma_{n'}) \right]. \tag{34}$$

Toshima [24] has reported an expression for the $ns \to n's$ charge-transfer amplitude in proton–hydrogen collisions which is a triple summation of one-dimensional integrals.

The expression for the differential cross section is

$$\frac{dQ}{d\Omega} = \frac{\mu_i K_f}{\mu_f K_i} |I|^2. \tag{35}$$

To obtain the total cross section we integrate the above expression numerically over the solid angle using an appropriate Gaussian quadrature method which takes proper account of the fact that the main contribution comes from very small scattering angles due to the

Table 1. Total cross sections (in πa_0^2) for the electron capture from ns state into $n's$ of atomic hydrogen for JS and DWB approximations (respectively). The numbers within the brackets (r), indicate that the cross sections are multiplied by 10^r.

Transition states	50 keV	100 keV	500 keV	1000 keV
$\phi_{1s \to 1s}$	0.519 26	0.732 21(−1)	0.998 29(−4)	0.291 80(−5)
	0.703 40	0.109 99	0.189 52(−3)	0.579 59(−5)
$\phi_{1s \to 2s}$	0.787 11(−1)	0.116 27(−1)	0.141 71(−4)	0.393 04(−6)
	0.104 02	0.169 39(−1)	0.269 05(−4)	0.780 32(−6)
$\phi_{1s \to 3s}$	0.242 78(−1)	0.361 51(−2)	0.430 14(−5)	0.118 10(−6)
	0.150 18	0.523 19(−2)	0.816 47(−5)	0.234 66(−6)
$\phi_{2s \to 1s}$	0.786 68(−1)	0.116 22(−1)	0.141 69(−4)	0.393 01(−6)
	0.103 96	0.169 32(−1)	0.269 01(−4)	0.780 25(−7)
$\phi_{2s \to 2s}$	0.181 22(−1)	0.194 75(−2)	0.202 73(−5)	0.530 75(−7)
	0.216 18(−1)	0.273 85(−2)	0.384 63(−5)	0.105 87(−6)
$\phi_{2s \to 3s}$	0.661 18(−2)	0.618 52(−3)	0.616 35(−6)	0.159 56(−7)
	0.756 56(−2)	0.861 66(−3)	0.116 89(−5)	0.318 55(−7)
$\phi_{3s \to 1s}$	0.242 62(−1)	0.361 32(−2)	0.430 06(−5)	0.118 09(−6)
	0.318 67(−1)	0.522 94(−2)	0.102 44(−4)	0.234 64(−6)
$\phi_{3s \to 2s}$	0.661 05(−2)	0.618 47(−3)	0.613 06(−6)	0.159 56(−7)
	0.756 42(−2)	0.861 59(−3)	0.318 03(−5)	0.318 54(−7)
$\phi_{3s \to 3s}$	0.254 78(−2)	0.198 17(−3)	0.187 44(−6)	0.479 73(−8)
	0.277 54(−2)	0.273 12(−3)	—	0.958 50(−8)

highly peaked angular distribution in the forward direction. So to give proper emphasis to very small scattering angles in our case, we have used the transformation

$$x = \frac{1}{2K_i^2 (1 - \cos\theta) + 1}.$$
(36)

For the 1s $\rightarrow$ n's transition the JS differential cross section shows minima in some small scattering angle for all energies of the incident proton. The total cross sections agree with the available results in the literature [2]. When we include the distortion potential over the JS approximation the values of the total cross section increase slightly. For ns $\rightarrow$ n's when $n \neq 1$ we have checked our results for the JS and DWB amplitudes for a few low-lying states against the corresponding results obtained by numerical integration. The results for total cross sections in different approximations have been displayed in table 1 for various energies of the incident proton. With the help of the computer program we have developed one can easily write down even the analytical expression of amplitude for the ns $\rightarrow$ n's transition.

4. Conclusion

An elegant analytic expression is presented for the evaluation of arbitrary higher-order derivatives of the Lewis integral which is frequently encountered in different branches of physics and quantum chemistry. The present closed form of the derivatives is considered to be better than some of the earlier approaches in this regard.

As a check of our formulation, we have made an application to the well studied problem of charge-transfer collisions in proton–hydrogen scattering. We have computed results for the ns $\rightarrow$ n's electron-capture processes in the JS and DWB approximations. The utility of our analytical expression can be seen from the fact that the results for the higher-order transitions in the DWB approximation are quite new and could not be attained earlier.

A generalization of the expression for the multi-order derivatives

$$\left[\left(\frac{\partial}{\partial\lambda_1}\right)\left(\frac{\partial}{\partial\lambda_2}\right)\cdots\left(\frac{\partial}{\partial\lambda_n}\right)\right]f(X_1(\lambda_1, \lambda_2, \cdots, \lambda_n),$$
$$X_2(\lambda_1, \lambda_2, \cdots, \lambda_n), \ldots, X_n(\lambda_1, \lambda_2, \cdots, \lambda_n))$$

is straightforward. In our forthcoming paper we shall consider transitions between arbitrary states when at least one of the initial and final states is nonspherical; the above-mentioned generalization will find an application in such cases.

Acknowledgments

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