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Evaluation of Some Integrals Required in Low-Energy Electron or Positron-Atom Scattering

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Various integrals containing either long-range terms or trigonometric functions arise in low-energy electron or positron-atom scattering problems. Analytical evaluation of such integrals becomes very difficult. Expressions are developed involving one final radial numerical integration, the other integrations being calculated analytically. These latter expressions may also be used in the optical potential method for scattering problems. The expressions are developed from expanding r_{ij}^{ν} in terms of Legendre polynomials. Using integrals for which analytical results are readily calculated for comparison purposes, it is found that at least ten significant figures are obtained from a 25-point Gauss–Laguerre quadrature.

Introduction

In the study of low-energy electron or positron-atom scattering problems, integrals of the form

$$I = (4\pi)^{-3} \int f(r_3)\, \chi \, d\tau \tag{1}$$

are encountered. r_3 denotes the magnitude of the projectile coordinate, $\mathbf{r}_3$, and $\int \cdots d\tau$ represents integration over the coordinates of the projectile and the target electrons. χ may contain factors of the form [1, 2, 3]

$$\chi = F_1(r_1)\, F_2(r_2)\, F_3(r_3)\, r_{23}^{\lambda} r_{13}^{\mu} r_{12}^{\nu} \tag{2}$$

with

$$F_a(r) = r^{m_a} e^{-\alpha_a r}. \tag{3}$$

r_1 and r_2 denote the magnitudes of the vector electron coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively, and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. Here m_a, ν, μ, and λ are integers $\geqslant -1$ and

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$\alpha_a > 0$. The function $f(r_3)$ may contain [1, 2, 3] either so-called long-range terms of the form

$$f(r_3) = (1 - e^{-\delta r_3})^3/r_3^2, \tag{4a}$$

or trigonometric terms such as

$$f(r_3) = (\sin kr_3)/kr_3, \tag{4b}$$

and

$$f(r_3) = (\cos kr_3)/kr_3, \tag{4c}$$

which arise from using variational methods in scattering problems at nonzero projectile energy.

Perkins [4] has developed explicit expressions for evaluating Eq. (1) when χ is given by Eq. (2) and $f(r_3) \equiv 1$. However, when $f(r_3)$ is given by, for example, Eq. (4), the analytic expressions of Perkins [4] become extremely difficult to evaluate. It is the purpose of this paper to develop analytic expressions for

$$Y(r_3) = (4\pi)^{-3} \int F_1(r_1)\, F_2(r_2)\, r_{23}^{\lambda} r_{13}^{\mu} r_{12}^{\nu}\, d\tau_1\, d\tau_2\, d\Omega_{r_3}, \tag{5}$$

where $d\tau_1$ and $d\tau_2$ are volume elements associated with $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively, and $d\Omega_{r_3}$ denotes the angular integration over the projectile vector r_3. I (Eq. (1)) is then given by

$$I = \int_0^\infty f(r_3)\, F_3(r_3)\, Y(r_3)\, r_3^2\, dr_3, \tag{6}$$

which can be evaluated numerically using, for example, Gaussian quadrature.

In some studies of collision problems, functions of the form of $Y(r_3)$ itself are needed to construct an optical potential. For example, in evaluating $\langle \psi_0(\mathbf{r}_1, \mathbf{r}_2) \mid H - E \mid \chi \rangle$, where $\psi_0(\mathbf{r}_1, \mathbf{r}_2)$ is the Hyllerras-type ground-state helium function, H and E are the Hamiltonian and energy of the system, respectively, an integration like Eq. (5) has to be carried out.

Analytical Integrals

Various integrals which will be used and which may be evaluated analytically are given below. Some of these integrals have been called either auxiliary or basic functions by other authors [5, 6].

$$A(F_a, N) = \int_0^\infty F_a(r)\, r^N\, dr, \tag{7}$$

$$B(F_a, N; x) = \int_0^x F_a(r)\, r^N\, dr, \tag{8}$$

$$D(F_a, N; x) = \int_x^\infty F_a(r)\, r^N\, dr, \tag{9}$$

$$E(F_a, M; F_b, N) = \int_0^\infty F_a(r)\, r^M\, dr \int_r^\infty F_b(t)\, t^N\, dt, \tag{10}$$

$$G(F_a, M; F_b, N; x) = \int_0^x F_a(r)\, r^M\, dr \int_0^r F_b(t)\, t^N\, dt, \tag{11}$$

$$H(F_a, M; F_b, N; x) = \int_0^x F_a(r)\, r^M\, dr \int_r^\infty F_b(t)\, t^N\, dt, \tag{12}$$

$$P(F_a, M; F_b, N; x) = \int_x^\infty F_a(r)\, r^M\, dr \int_0^r F_b(t)\, t^N\, dt, \tag{13}$$

$$Q(F_a, M; F_b, N; x) = \int_x^\infty F_a(r)\, r^M\, dr \int_r^\infty F_b(t)\, t^N\, dt. \tag{14}$$

General Expressions

r_{12}^ν may be expanded, using Perkins' notation [4], in the form

$$r_{12}^\nu = \sum_{q=0}^{L_1} P_q(\cos\theta_{12}) \sum_{k=0}^{L_2} C_{\nu,q,k} s_{12}^{q+2k} g_{12}^{\nu-q-2k}, \tag{15}$$

where s_{12}, g_{12} denote the smaller and greater of r_1 and r_2, respectively; the P's are the Legendre polynomials, θ_{12} being the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$; the C's are the same coefficients as those derived by Perkins [4]. If ν is even, $L_1 = \nu/2$, $L_2 = \nu/2 - q$; if ν is odd, $L_1 = \infty$, $L_2 = [(\nu+1)/2] \equiv$ integral part of $(\nu+1)/2$. After expressing r_{23}^λ, r_{13}^μ and r_{12}^ν in the form of Eq. (15) and performing the angular integrations, Eq. (5) becomes

$$Y(r_3) = \sum_{q=0}^{\infty} (2q+1)^{-2} \sum_{i=0}^{[(\lambda+1)/2]} C_{\lambda,q,i} \sum_{j=0}^{[(\mu+1)/2]} C_{\mu,q,j} \sum_{k=0}^{[(\nu+1)/2]} C_{\nu,q,k}$$

$$\times \int s_{12}^{q+2k} g_{12}^{\nu-q-2k} g_{13}^{\mu-q-2j} s_{13}^{q+2j} s_{23}^{q+2i} g_{23}^{\lambda-q-2i} r_1{}^2 r_2{}^2 F_1(r_1)\, F_2(r_2)\, dr_1\, dr_2\,. \tag{16}$$

The r_1 integration may be divided into three intervals: 0 to s_{23}; s_{23} to g_{23}; g_{23} to ∞; while the r_2 integration may be divided into two intervals: 0 to r_3; r_3 to ∞.

Using this integration scheme, Eq. (16) becomes

$$Y(r_3) = \sum_{q=0}^{\infty} (2q+1)^{-2} \sum_{i=0}^{[(\lambda+1)/2]} C_{\lambda,q,i} \sum_{j=0}^{[(\mu+1)/2]} C_{\mu,q,j} \sum_{k=0}^{[(\nu+1)/2]}$$

$$\times C_{\nu,q,k} \Big[r_3^{\lambda+\mu-2q-2i-2j} \int_0^{r_3} r_2^{2+\nu+2i-2k} F_2(r_2)\, dr_2 \int_0^{r_2} r_1^{2+2q+2j+2k} F_1(r_1)\, dr_1$$

$$+ r_3^{\lambda+\mu-2q-2i-2j} \int_0^{r_3} r_2^{2+2q+2i+2k} F_2(r_2)\, dr_2 \int_{r_2}^{r_3} r_1^{2+\nu+2j-2k} F_1(r_1)\, dr_1$$

$$+ r_3^{\lambda-2i+2j} \int_0^{r_3} r_2^{2+2q+2i+2k} F_2(r_2)\, dr_2 \int_{r_3}^{\infty} r_1^{2+\mu+\nu-2q-2j-2k} F_1(r_1)\, dr_1$$

$$+ r_3^{\mu+2i-2j} \int_{r_3}^{\infty} r_2^{2+\lambda+\nu-2q-2i-2k} F_2(r_2)\, dr_2 \int_0^{r_3} r_1^{2+2q+2j+2k} F_1(r_1)\, dr_1$$

$$+ r_3^{2q+2i+2j} \int_{r_3}^{\infty} r_2^{2+\lambda+\nu-2q-2i-2k} F_2(r_2)\, dr_2 \int_{r_3}^{r_2} r_1^{2+\mu-2j+2k} F_1(r_1)\, dr_1$$

$$+ r_3^{2q+2i+2j} \int_{r_3}^{\infty} r_2^{2+\lambda-2i+2k} F_2(r_2)\, dr_2 \int_{r_2}^{\infty} r_1^{2+\mu+\nu-2q-2j-2k} F_1(r_1)\, dr_1 \Big]. \tag{17}$$

For large values of q, the power of r_1 in the last integral of Eq. (17) becomes negative. To avoid this difficulty, the following identity is used to change the order of integration between r_1 and r_2:

$$\int_a^b h(r_2)\, dr_2 \int_{r_2}^b g(r_1)\, dr_1 = \int_a^b g(r_1)\, dr_1 \int_a^{r_1} h(r_2)\, dr_2. \tag{18}$$

Using the functions defined in Eqs. (7)–(14) together with Eq. (18), Eq. (5) becomes

$$Y(r_3) = \sum_{q=0}^{\infty} (2q+1)^{-2} \sum_{i=0}^{[(\lambda+1)/2]} C_{\lambda,q,i} \sum_{j=0}^{[(\mu+1)/2]} C_{\mu,q,j} \sum_{k=0}^{[(\nu+1)/2]}$$

$$\times C_{\nu,q,k} [r_3^{\lambda+\mu-2q-2i-2j} \{G(F_2, 2+\nu+2i-2k; F_1, 2+2q+2j+2k; r_3)$$

$$+ G(F_1, 2+\nu+2j-2k; F_2, 2+2q+2i+2k; r_3)\}$$

$$+ r_3^{\lambda-2i+2j} B(F_2, 2+2q+2i+2k; r_3)$$

$$\times D(F_1, 2+\mu+\nu-2q-2j-2k; r_3)$$

$$+ r_3^{\mu+2i-2j} B(F_1, 2+2q+2j+2k; r_3)$$

$$\times D(F_2, 2+\lambda+\nu-2q-2i-2k; r_3)$$
$$+ r_3^{2q+2i+2j}\{D(F_2, 2+\lambda+\nu-2q-2i-2k; r_3)$$
$$\times D(F_1, 2+\mu-2j+2k; r_3)$$
$$- Q(F_2, 2+\lambda+\nu-2q-2i-2k; F_1, 2+\mu-2j+2k; r_3)$$
$$+ D(F_1, 2+\mu+\nu-2q-2j-2k; r_3)\, D(F_2, 2+\lambda-2i+2k; r_3)$$
$$- Q(F_1, 2+\mu+\nu-2q-2j-2k; F_2, 2+\lambda-2i+2k; r_3)\}]. \quad (19)$$

Special Cases

The general expression for $Y(r_3)$ given in Eq. (19) may be simplified, as in the work of Perkins [4], in the special cases where any of the integers λ, ν, μ are even. These cases will be given here.

(i) ν *is even.*

$$Y(r_3) = \sum_{q=0}^{\nu/2} (2q+1)^{-2} \sum_{i=0}^{[(\lambda+1)/2]} C_{\lambda,q,i} \sum_{j=0}^{[(\mu+1)/2]} C_{\mu,q,j} \sum_{k=0}^{\nu/2-q}$$
$$\times C_{\nu,q,k}[r_3^{\lambda+\mu-2q-2i-2j} B(F_2, 2+2q+2i+2k; r_3)$$
$$\times B(F_1, 2+\nu+2j-2k; r_3) + r_3^{\lambda+2j-2i} B(F_2, 2+2q+2i+2k; r_3)$$
$$\times D(F_1, 2+\mu+\nu-2q-2j-2k; r_3) + r_3^{\mu+2i-2j}$$
$$\times B(F_1, 2+2q+2j+2k; r_3)\, D(F_2, 2+\lambda+\nu-2q-2i-2k; r_3)$$
$$+ r_3^{2q+2i+2j} D(F_2, 2+\lambda+\nu-2q-2i-2k; r_3)$$
$$\times D(F_1, 2+\mu-2j+2k; r_3)]. \quad (20)$$

(ii) μ *is even.*

$$Y(r_3) = \sum_{q=0}^{\mu/2} (2q+1)^{-2} \sum_{i=0}^{[(\lambda+1)/2]} C_{\lambda,q,i} \sum_{j=0}^{\mu/2-q} C_{\mu,q,j} \sum_{k=0}^{[(\nu+1)/2]}$$
$$\times C_{\nu,q,k}[r_3^{\lambda+\mu-2q-2i-2j}\{G(F_2, 2+\nu+2i-2k; F_1, 2+2q+2j+2k; r_3)$$
$$+ H(F_2, 2+2q+2i+2k; F_1, 2+\nu+2j-2k; r_3)\}$$
$$+ r_3^{\mu+2i-2j}\{P(F_2, 2+\lambda+\nu-2q-2i-2k; F_1, 2+2q+2j+2k; r_3)$$
$$+ Q(F_2, 2+\lambda-2i+2k; F_1, 2+\nu+2j-2k; r_3)\}]. \quad (21)$$

(iii) *λ is even.* Due to the symmetry of the two electrons at $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively, the expression for $Y(r_3)$ in this case is given by Eq. (21) interchanging F_1 with F_2 and μ with λ.

(iv) *μ and ν are both even.*

$$Y(r_3) = \sum_{q=0}^{\min(\nu/2,\mu/2)} (2q+1)^{-2} \sum_{i=0}^{[(\lambda+1)/2]} C_{\lambda,q,i} \sum_{j=0}^{\mu/2-q} C_{\mu,q,j} \sum_{k=0}^{\nu/2-q}$$
$$\times C_{\nu,q,k}[r_3^{\lambda+\mu-2q-2i-2j} B(F_2, 2+2q+2i+2k; r_3)\, A(F_1, 2+\nu+2j-2k)$$
$$+ r_3^{\mu+2i-2j} D(F_2, 2+\lambda+\nu-2q-2i-2k; r_3)\, A(F_1, 2+2q+2j+2k)]. \tag{22}$$

Where $\min(\nu/2, \mu/2)$ denotes the minimum of $\nu/2$ and $\mu/2$.

(v) *λ and ν are both even.* Again, due to symmetry of the two electrons at $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively, the expression for $Y(r_3)$ in this case is given by Eq. (22) interchanging F_1 with F_2 and μ with λ.

(vi) *λ and μ are both even.*

$$Y(r_3) = \sum_{q=0}^{\min(\mu/2,\lambda/2)} (2q+1)^{-2} \sum_{i=0}^{\lambda/2-q} C_{\lambda,q,i} \sum_{j=0}^{\mu/2-q} C_{\mu,q,j} \sum_{k=0}^{[(\nu+1)/2]}$$
$$\times C_{\nu,q,k} r_3^{\lambda+\mu-2q-2i-2j} [E(F_1, 2+2q+2j+2k; F_2, 2+\nu+2i-2k)$$
$$+ E(F_2, 2+2q+2i+2k; F_1, 2+\nu+2j-2k)]. \tag{23}$$

(vii) *λ, μ and ν are all even.*

$$Y(r_3) = \sum_{q=0}^{\min(\lambda/2,\mu/2,\nu/2)} (2q+1)^{-2} \sum_{i=0}^{\lambda/2-q} C_{\lambda,q,i} \sum_{j=0}^{\mu/2-q} C_{\mu,q,j} \sum_{k=0}^{\nu/2-q} C_{\nu,q,k}$$
$$\times r_3^{\lambda+\mu-2q-2i-2j} A(F_2, 2+\nu+2i-2k)\, A(F_1, 2+2q+2j+2k). \tag{24}$$

Evaluation of Analytical Integrals

The analytical determination of $A(F_a, N)$ is straightforward. Since $E(F_a, M; F_b, N)$ appears in Eq. (23) with M and N both $\geqslant 0$, it may be expressed in terms of the integrals defined in Eqs. (7) and (9). Similarly the integrals listed in Eqs. (11)–(14) may be expressed in terms of the integrals defined in Eqs. (7)–(9).

$B(F_a, N; x)$ may be evaluated by means of a recursion relation [5, 6]. However, round-off errors become severe in using the recursion relation for certain values of x and another method of evaluation must be used [5, 6]. When the power of r

is positive, a recursion relation for $D(F_a, N; x)$ may be used throughout the entire range of x without significant round-off errors accumulating [6]. For negative powers of r, $D(F_a, N; x)$ may be related to the exponential integral through a recursion relation [7]. Cody and Thacher [8] have developed accurate rational Chebyshev approximations for the exponential integral. It has been found [7] that the recursion relation for negative powers of r may result in serious round-off errors accumulating for certain values of both x and N. In such cases, alternative procedures have been developed [7, 9]. However, in the present work, it was found that the contributions of such terms to the total integral, I, were insignificant.

TABLE I

Sample of Integrals Used to Test the Accuracy of the Various Formulae

$$I = (4\pi)^{-3} \int e^{-\alpha_1 r_1} e^{-\alpha_2 r_2} e^{-\alpha_3 r_3} r_1^{m_1} r_2^{m_2} r_3^{m_3} r_{23}^{\lambda} r_{13}^{\mu} r_{12}^{\nu} \, d\tau$$

α_1	α_2	α_3	m_1	m_2	m_3	λ	μ	ν	Values of I using 25-point Gauss–Laguerre quadrature	Values of I using expressions of Perkins [4]
5.72	4.26	4.26	0	0	0	−1	1	1	.690670359335 $E-05$	.690670359371 $E-05$
5.72	4.26	4.26	2	1	1	1	1	1	.339516939432 $E-05$	.339516939432 $E-05$
5.72	5.72	2.80	2	1	1	3	3	3	.103057681192 $E-02$	.103057681192 $E-02$
4.26	4.26	5.72	2	1	1	5	5	5	.197989903162 $E+00$	.197989903162 $E+00$
5.72	4.26	4.26	0	1	1	0	1	1	.433603504031 $E-05$	.433603504031 $E-05$
2.80	4.26	5.72	1	0	2	3	0	−1	.187402878185 $E-04$	.187402878185 $E-04$
2.80	4.26	5.72	2	1	0	1	−1	2	.844226266354 $E-04$	.844226266354 $E-04$
2.80	5.72	5.72	2	0	0	0	0	−1	.108435060844 $E-04$	.108435060844 $E-04$
5.72	5.72	2.80	0	0	2	0	−1	2	.774239416524 $E-05$	.774239416441 $E-05$
2.80	4.26	5.72	0	2	1	−1	2	0	.168795448669 $E-04$	.168795448669 $E-04$
5.72	5.72	2.80	0	0	2	0	0	0	.159259337056 $E-04$	.159259337056 $E-04$

The accuracy of the formulae presented in this paper were tested using various integrals for which the analytical expressions of Perkins [4] could be readily used. It was found that a 32-point Gauss–Laguerre quadrature gave at least 13 significant figures in the final answers for all cases except when ν, μ and λ were all odd integers. Using a 25-point quadrature resulted in an accuracy of at least ten significant figures, while a 16-point quadrature gave at least six significant figures. For the

TABLE II

Convergence Behavior of Typical Integrals When ν, μ, λ Are All Odd

$$I = (4\pi)^{-3} \int e^{-\alpha_1 r_1} e^{-\alpha_2 r_2} e^{-\alpha_3 r_3} r_1^{m_1} r_2^{m_2} r_3^{m_3} r_{23}^{\lambda} r_{13}^{\mu} r_{12}^{\nu} \, d\tau = \sum_{q=0}^{\infty} J_q$$

α_1	α_2	α_3	m_1	m_2	m_3	λ	μ	ν
5.72	4.26	4.26	0	0	0	−1	1	1

q	J_q using 25-point Gauss–Laguerre quadrature	J_q using the expressions of Perkins [4]
0	.681417026290 $E-05$	.681417026289 $E-05$
1	.009160399879 $E-05$	.009160399887 $E-05$
2	.000086633829 $E-05$	.000086633821 $E-05$
3	.000005397857 $E-05$	.000005397857 $E-05$
4	.000000705323 $E-05$	.000000705324 $E-05$
5	.000000140240 $E-05$	.000000140240 $E-05$
6	.000000036673 $E-05$	.000000036673 $E-05$
7	.000000011640 $E-05$	.000000011640 $E-05$
8	.000000004270 $E-05$	.000000004270 $E-05$
9	.000000001752 $E-05$	.000000001752 $E-05$
10	.000000000786 $E-05$	.000000000786 $E-05$
11	.000000000379 $E-05$	.000000000379 $E-05$
12	.000000000195 $E-05$	.000000000195 $E-05$
13	.000000000105 $E-05$	.000000000105 $E-05$
14	.000000000059 $E-05$	.000000000059 $E-05$
15	.000000000035 $E-05$	.000000000035 $E-05$
16	.000000000023 $E-05$	.000000000021 $E-05$
17	.000000001322 $E-05$	.000000000013 $E-05$
18	.000000002742 $E-05$	.000000000008 $E-05$
19	−.000000001180 $E-05$	.000000000006 $E-05$
20		.000000000004 $E-05$
21		.000000000003 $E-05$
22		.000000000002 $E-05$
23		.000000000001 $E-05$
24		.000000000001 $E-05$
25		.000000000001 $E-05$

Table continued

TABLE II (*continued*)

α_1	α_2	α_3	m_1	m_2	m_3	λ	μ	ν
4.26	4.26	5.72	2	1	1	5	5	5

q	J_q using 25-point Gauss–Laguerre quadrature	J_q using the expressions of Perkins [4]
0	.280791345363 $E + 00$	.280791345363 $E + 00$
1	−.084479705809 $E + 00$	−.084479705809 $E + 00$
2	.001678931336 $E + 00$	.001678931336 $E + 00$
3	−.000000667559 $E + 00$	−.000000667559 $E + 00$
4	−.000000000169 $E + 00$	−.000000000169 $E + 00$
5	−.000000000001 $E + 00$	−.000000000001 $E + 00$

cases where the integers ν, μ, and λ are all odd, the 32-point, 25-point, and 16-point quadratures gave an accuracy of at least ten, ten, and nine significant figures, respectively. A 40-point quadrature gave the same results as the 32-point quadrature. A sample table of test integrals is given in Table I where the numbers are rounded off to 12 significant figures. Here the results using a 25-point quadrature are compared with those obtained using the expressions of Perkins [4]. Since the case where the integers ν, μ, and λ are all odd involve an infinite sum over the variable q, the individual contributions for each value of q to the final answer are given in Table II for two cases. When q is large, differencing errors in using Eq. (19) completely dominate the contributions to the integral I. This occurs in one of the examples in Table II when q is greater than 16.

All the computations were performed using the Control Data Corporation Cyber 73/14 computer system at the University of Western Ontario. This computer has a 60-bit word length, giving 14 significant figures for single precision arithmetic.

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