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Note

Closed Form Expressions for an Integral Involving the Coulomb Potential

Expressions for an integral related to the Coulomb potential are given. The expressions are in terms of logarithms and polynomials or logarithms and sums of Legendre polynomials. Identities relating an infinite sum of Legendre polynomials to a finite sum of Legendre polynomials can be deduced. This expression can be used in the domain to $t \to 1$, $z \to 1$ where quadrature fails. © 1986 Academic Press, Inc.

The integral,

$$I_n = \int t^n / R \, dt; \qquad R = (1 - 2zt + t^2)^{1/2}, \quad |z| \leqslant 1, \; n \in \mathbb{Z}^+$$

arises when expanding the potential term of a conservative field, such as the Coulomb interaction in atomic and molecular systems or the gravitational interaction in planetary systems.

Explicit forms for the first four n values and a procedure to calculate the integral for any particular value of n are given in [1]. The general form can be calculated from the recurrence relation [2] using standard methods for solving second order difference equations with variable coefficients [3]. The solution, in terms of Legendre polynomials, is

$$I_n = P_n(z)\, I_0 + R \sum_{i=0}^{n-1} t^i \sum_{k=i}^{n-1} \frac{P_n(z)\, P_i(z)}{(k+1)\, P_k(z)\, P_{k+1}(z)}, \tag{1}$$

where

$$I_0 = \begin{cases} \operatorname{arcsinh}[(t-z)(1-z^2)^{-1/2}], & z \neq 1 \\ -\ln[1-t], & z = 1. \end{cases}$$

An alternative expression can be deduced by assuming a solution of the form

$$I_n = P_n(z)\, I_0 + R p_n(t, z), \tag{2}$$

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where $p_n(t, z)$ is a polynomial of degree $n-1$ in z and t. Substituting into the recurrence relation gives the following expression for the polynomial part,

$$p_n(t, z) = \pi^{-1} \sum_{m=0}^{n-1} t^{n-m-1} \Gamma(n-m)/n! \sum_{a=0}^{[m/2]} \binom{m-a}{a} (2z)^{m-2a}(-1)^a$$
$$\times \sum_{i=0}^{a} \binom{a}{i} \Gamma(n-i+1/2)[\Gamma(i+1/2)]^2/\Gamma(n-m+i+1/2). \tag{3}$$

Hence we have a closed form for the integral in terms of a logarithm and a polynomial in t and z. By equating the coefficients of t in (1) and (3) we obtain an expression for a finite sum of products of Legendre polynomials. Furthermore we note that if a is a positive integer, then

$$\sum_{k=0}^{\infty} x^k P_k(z)/(k+a) = x^{-a} \int_0^x t^{a-1}/R \, dt, \qquad \text{where} \quad \begin{cases} |z| \leqslant 1 & \text{if } 0 \leqslant x < 1 \\ -1 \leqslant z < 1 & \text{if } x = 1 \end{cases}$$

and so we have a closed form for an infinite sum over Legendre polynomials. If $r_<$ is the distance to the nearest of a pair of particles, $r_>$ the distance to the other and ω the angle between them then we can interpret x as $r_</r_>$, z as $\cos \omega$ and R as the interparticle distance.

The integral I_n is encountered when solving directly the Schrodinger equation for few-particle systems interacting with the Coulomb potential. For example the expansion occurs in the ^1S states of helium constructed using recurrence relations [4]. In algebraic work of his type the expansion (2) is convenient because it is readily manipulated using algebraic computing programs. It is also helpful in numerical studies of the form of wavefunctions near singularities in Coulomb potentials.

Equation (2) splits I_n into two components, an infinite series (arcsinh or ln), and a polynomial of degree $n-1$. The polynomial part can be evaluated in $O(n^3)$ multiplications and divisions. For small n (~ 10), Eq. (2) and quadrature involve computations of the same order. In the limit of $t \to 1$, $z \to 1$, i.e., the coalescence of the two particles, the integrand and the integral are singular. Near the singularity quadrature will be inaccurate due to slow convergence but (2) is still easily calculated. At the singularity quadrature fails but (2) can still be used to extract information as the singularity is expressed as a logarithm.

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