COULOMB WAVE FUNCTIONS IN TERMS OF JACOBI POLYNOMIAL AND GENERALIZED CONFLUENT HYPERGEOMETRIC FUNCTIONS

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Analytic expansions of both regular and irregular Coulomb wave functions for all values of angular momentum quantum number L as a product of Jacobi and generalized confluent hypergeometric functions are evaluated. They are deduced with the help of a new expansion formula for Kampé de Fériet function established in this paper and the orthogonal property of Jacobi polynomials.

1. INTRODUCTION

For the study of nuclear reactions involving positively charged particles like protons, deutrons, α particles and heavy ions the knowledge of Coulomb wave functions is of paramount importance. The regular and irregular forms of these functions may be expressed in terms of Whittaker functions by the equations (Abramowitz 1952, Morse and Feshbach 1953)

$$F_L(\eta, \rho) = \tfrac{1}{2} \frac{Q_L(\eta)(i)^{-L-1}}{(2L+1)!} M_{i\eta,\, L+\frac{1}{2}}(2i\rho), \qquad (1.1)$$

$$G_L(\eta, \rho) = \frac{1}{Q_L(\eta)} \operatorname{Re} \left(\Gamma(L+1-i\eta) i^L W_{i\eta,\, L+\frac{1}{2}}(2i\rho)\right), \qquad (1.2)$$

$$Q_L(\eta) = \left\{ (1^2+\eta^2)(2^2+\eta^2) \ldots (L^2+\eta^2) \frac{2\pi\eta}{e^{2\pi\eta}-1} \right\}^{\frac{1}{2}}, \qquad (1.3)$$

where L is the orbital angular momentum quantum number; $\eta = zz'e^2/\hbar v$; $\rho = \mu vr/\hbar$; v being the relative velocity of the colliding particles, r is the distance between them, μ is the reduced mass and Ze, $Z'e$ being their charges.

The complete review of the various treatments of these functions and their tables has been given by Abramowitz (1952), Abramowitz and Stegun (1965) and Lukyanov *et al.* (1965). These tables are compiled for the computation of the Coulomb wave functions on the surface of the nucleus, i.e. for calculations in the theory of nuclear reactions that are accompanied by the formation of a compound nucleus.

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Abramowitz (1954) evaluated for low energy particles expansions of these functions in terms of Bessel functions. For high energy particles the Bessel function expansion for the regular functions for all values of L had been obtained by Meligy (1956). Meligy and Gazzy (1962) obtained for high energy particles the expansions of both regular and irregular Coulomb wave functions for all values of L in terms of spherical Bessel functions.

The object of the present paper is to evaluate expansions as a product of Jacobi and generalized confluent hypergeometric functions for all values of L for both regular and irregular wave functions.

For deriving the expansions for the Coulomb wave functions, we have first established a desired integral in Section 2. In Section 3, we have obtained an expansion formula for Kampé de Fériet function using the integral obtained in Section 2 and the orthogonal property of Jacobi polynomials. Finally, in Section 4, we have expressed for all values of L the regular and irregular wave functions in terms of Jacobi and generalized confluent hypergeometric functions.

We made use of the familiar abbreviation

$$(a)_m = \frac{\Gamma(a+m)}{\Gamma(a)} = a(a+1)\ldots(a+m-1)$$

and in what followed for the sake of brevity we expressed the Kampé de Fériet function in the notations of Burchnall and Chaundy (1941)

$$F\left[\begin{matrix}(a),\,(a'):(c);\;(c');\\(b),\,(b'):(d);\;(d');\end{matrix}\;x,\,y\right] = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{((a))_{m+n}((a'))_{m+n}((c))_m((c'))_n x^m y^n}{((b))_{m+n}((b'))_{m+n}((d))_m((d'))_n(m)!\,(n)!}$$

where, $A+A'+C \leqslant B+B'+D$ and $C'+A+A' \leqslant B+B'+D'$.
Further (a) is taken to denote the sequence of A parameters

$a_1,\ a_2,\ \ldots,\ a_A$, that is, unless stated otherwise there are A of a parameters, A' of a' parameters and so on. Thus $((a))_m$ is to be interpreted as $\prod_{j=1}^{A}(a_j)_m$, with similar interpretations for $((a'))_m$, etc.

2. Derivation of the Integral

We first establish the following integral required for our desired expansion

$$\int_0^1 \rho^{\delta}(1-\rho)^{\beta}P_n^{(\alpha,\beta)}(1-2\rho)F\left[\begin{matrix}(a),\,(a'):(c);\;(c');\\(b),\,(b'):(d);\;(d');\end{matrix}\;x\rho,\,y\rho\right]d\rho$$

$$= \frac{\Gamma(1+\delta)\,\Gamma(1+\beta+n)\,\Gamma(\alpha-\delta+n)}{(n)!\,\Gamma(\alpha-\delta)\,\Gamma(\beta+\delta+n+2)}F\left[\begin{matrix}1+\delta, & 1+\delta-\alpha, & (a),(a'):(c);(c');\\1+\delta-\alpha-n, & \beta+\delta+n+2, & (b),(b'):(d);(d');\end{matrix}\;x,\,y\right] \quad \ldots (2.1)$$

with conditions of validity as
$A+A'+C \leqslant B+B'+D, A+A'+C' \leqslant B+B'+D'$, Re $(\delta) > -1$, Re $(\beta) > -1$, and $P_n^{(\alpha,\beta)}(1-2\rho)$ is the Jacobi polynomial.

For evaluating the integral, we express the Kampé de Fériet function on the L.H.S. of (2.1) in the series form and then change the order of integration and summation which is justified (Carslaw 1930). Finally, solving the inner integral with the help of formula (Erdélyi 1954) and simplifying, we get the desired integral.

3. Expansion of the Kampé de Fériet Function

The expansion to be established is

$$\rho^\delta F\left[\begin{matrix}(a), (a'):(c);\ (c');\\ (b), (b'):(d);\ (d');\end{matrix}\ x\rho,\ y\rho\right] = \sum_{r=0}^{\infty} M_r P_r^{(\alpha,\beta)}(1-2\rho)$$
$$\times F\left[\begin{matrix}1+\delta+\alpha, & 1+\delta, & (a), (a'):(c);\ (c');\\ 1+\delta-r, & \beta+\alpha+\delta+r+2, & (b), (b'):(d);\ (d');\end{matrix}\ x, y\right] \quad .. \quad (3.1)$$

where

$$M_r = \frac{\Gamma(1+\alpha+\delta)\,\Gamma(r-\delta)(\alpha+\beta+2r+1)\,\Gamma(1+\alpha+\beta+r)}{\Gamma(-\delta)\,\Gamma(\alpha+\beta+\delta+r+2)\,\Gamma(1+\alpha+r)} \quad .. \quad (3.2)$$

provided that,
$A+A'+C \leqslant B+B'+D$, $A+A'+C' \leqslant B+B'+D'$, Re $(\rho+\alpha) > -1$, Re $(\alpha) > -1$ Re $(\beta) > -1$ and $\delta \geqslant 0$.

Proof: To prove (3.1), let

$$f(\rho) = \rho^\delta F\left[\begin{matrix}(a), (a'):(c);\ (c');\\ (b), (b'):(d);\ (d');\end{matrix}\ x\rho,\ y\rho\right] = \sum_{r=0}^{\infty} A_r P_r^{(\alpha,\beta)}(1-2\rho). \quad .. \quad (3.3)$$

Equation (3.3) is valid since $f(\rho)$ is continuous and of bounded variation in the open interval (0, 1) where $\delta \geqslant 0$.

Multiplying both sides of (3.3) by $\rho^\alpha(1-\rho)^\beta P_n^{(\alpha,\beta)}(1-2\rho)$ and integrating between the limits 0 to 1, we have

$$\int_0^1 \rho^{\delta+\alpha}(1-\rho)^\beta P_n^{(\alpha,\beta)}(1-2\rho) F\left[\begin{matrix}(a), (a'):(c);\ (c');\\ (b), (b'):(d);\ (d');\end{matrix}\ x\rho,\ y\rho\right] d\rho$$
$$= \sum_{r=0}^{\infty} A_r \int_0^1 \rho^\alpha(1-\rho)^\beta P_n^{(\alpha,\beta)}(1-2\rho) P_r^{(\alpha,\beta)}(1-2\rho)\, d\rho. \quad .. \quad (3.4)$$

Now using (2.1) and the orthogonal property of Jacobi polynomials (Erdélyi 1954), viz.

$$\int_0^1 \rho^\alpha(1-\rho)^\beta P_n^{(\alpha,\beta)}(1-2\rho) P_m^{(\alpha,\beta)}(1-2\rho)\, d\rho \begin{cases} = 0 & m \neq n \\ = \dfrac{\Gamma(1+\alpha+n)\,\Gamma(1+\beta+n)}{(n)!\,(\alpha+\beta+2n+1)\Gamma(\alpha+\beta+n+1)} & (m = n) \end{cases} \quad .. \quad (3.5)$$

we get

$$A_n = M_n F\begin{bmatrix}1+\delta+\alpha, & 1+\delta & (a), (a') : (c); (c'); \\ 1+\delta-n, & \alpha+\beta+\delta+n+2, & (b), (b') : (d); (d'); \end{bmatrix} x, y \quad .. \quad (3.6)$$

here M_n is obtained by putting n for r in eqn. (3.2).

Hence the expansion (3.1) follows from (3.3) and (3.6) immediately.

4. The Expansions of the Coulomb Functions

In eqn. (3.1) if a, a', b and b' are chosen such that $a = b$ and $a' = b'$, the double hypergeometric function on left breaks up into the product of two generalized hypergeometric functions.

Thus

$$\rho^\delta {}_CF_D\begin{bmatrix}(c); \\ (d); \end{bmatrix} x\rho \Big] {}_CF_D\begin{bmatrix}(c'); \\ (d'); \end{bmatrix} y\rho \Big] = \sum_{r=0}^{\infty} M_r P_r^{(\alpha,\beta)}(1-2\rho)$$

$$\times F\begin{bmatrix}1+\delta+\alpha, & 1+\delta & : (c); (c'); \\ 1+\delta+r, & \alpha+\beta+\delta+r+2 & : (d); (d'); \end{bmatrix} x, y \Big] \quad .. \quad .. \quad (4.1)$$

The conditions of validity for (4.1) are the same (with $A = B$, $A' = B'$) as for eqn. (3.1).

Further it is well known that for $y = 0$

$$F\begin{bmatrix}(a), (a') : (c); (c'); \\ (b), (b') : (d); (d'); \end{bmatrix} x, y \Big] = {}_{A+A'+C}F_{B+B'+D}\begin{bmatrix}(a), (a'), (c); \\ (b), (b'), (d); \end{bmatrix} x \Big]. \quad .. \quad (4.2)$$

Now the special case $A = A' = B = B' = 0$ for (3.1) yields

$$\rho^\delta {}_CF_D\begin{bmatrix}(c); \\ (d); \end{bmatrix} x\rho \Big] = \sum_{r=0}^{\infty} M_r \, {}_{C+2}F_{D+2}\begin{bmatrix}1+\delta+\alpha, & 1+\delta, & (c); \\ 1+\delta+r, & \alpha+\beta+\delta+r+2, & (d); \end{bmatrix} x \Big] \times P_r^{(\alpha,\beta)}(1-2\rho).$$

.. (4.3)

Equation (4.3) is valid under the same conditions as for equation (3.1) with $A = A' = B = B' = C' = D' = 0$.

Now setting $C = D = 1$, $c_1 = 1+L-i\eta$, $d_1 = 2L+2$, $x = 2i$ in eqn. (4.3), we get

$$\rho^\delta {}_1F_1\begin{bmatrix}1+L-i\eta; \\ 2L+2; \end{bmatrix} 2i\rho \Big] = \sum_{r=0}^{\infty} M_r P_r^{(\alpha,\beta)}(1-2\rho)$$

$$\times {}_3F_3\begin{bmatrix}1+\alpha+\delta, & 1+\delta, & 1+L-i\eta; \\ 1+\delta-r, & \alpha+\beta+\delta+r+2, & 2L+2; \end{bmatrix} 2i \Big]. \quad (4.4)$$

Now with the help of eqn. (1.1), we get finally the following expansion for regular Coulomb wave functions in terms of Jacobi and generalized confluent hypergeometric functions

$$F_L(\eta, \rho) = \frac{e^{-i\rho} Q_L(\eta) 2^L \rho^{1+L-\delta}}{(2L+1)!} \sum_{r=0}^{\infty} M_r P_r^{(\alpha,\beta)}(1-2\rho)$$

$$\times {}_3F_3\begin{bmatrix}1+\alpha+\delta, & 1+\delta, & 1+L-i\eta; \\ 1+\delta-r, & \alpha+\beta+\delta+r+2, & 2+2L; \end{bmatrix} 2i \Big] \quad .. \quad (4.5)$$

provided that Re $(\alpha+\delta) > -1$ Re $(\beta) > -1$, Re $(\alpha) > -1$ and $\delta \geqslant 0$.

For evaluating the corresponding expansion formula for irregular Coulomb wave function, we rewrite eqn. (1.2) in the following form

$$G_L(\eta, \rho) = \frac{1}{Q_L(\eta)} \text{Re} \left\{ \Gamma(1+L-i\eta) i^L \left[\frac{\Gamma(-1-2L)}{\Gamma(-L-i\eta)} M_{i\eta, L+\frac{1}{2}}(2i\rho) + \frac{\Gamma(1+2L)}{\Gamma(1+L-i\eta)} M_{i\eta, -L-\frac{1}{2}}(2i\rho) \right] \right\}. \quad \ldots \quad (4.6)$$

Now from eqn. (1.1)

$$G_L(\eta, \rho) = \text{Re} \left[\frac{\Gamma(1+L-i\eta) 2i(-1)^L \Gamma(-1-2L) \Gamma(2L+2)}{\Gamma(-L-i\eta)[Q_L(\eta)]^2} F_L(\eta, \rho) + \frac{\Gamma(1+L-i\eta) 2\, \Gamma(1+2L)\, \Gamma(-2L)}{\Gamma(1+L-i\eta) Q_L(\eta) Q_{-L-1}(\eta)} F_{-L-1}(\eta, \rho) \right]. \quad \ldots \quad (4.7)$$

Thus from eqn. (4.5), we finally get the following expansion formula for the irregular Coulomb wave functions:

$$G_L(\eta, \rho) = \text{Re} \left[\frac{\Gamma(1+L-i\eta) e^{-i\rho} \rho^{-\delta}}{Q_L(\eta)} \left\{ \frac{(2\rho)^{1+L} i(-1)^L \Gamma(-1-2L)}{\Gamma(-L-i\eta)} \sum_{r=0}^{\infty} M_r P_r^{(\alpha,\beta)}(1-\rho) \right. \right.$$
$$\times {}_3F_3 \left[\begin{matrix} 1+\delta+\alpha, & 1+\delta, & 1+L-i\eta; \\ 1+\delta+r, & \alpha+\beta+\delta+r+2, & 2+2L; \end{matrix} 2i \right]$$
$$\left. \left. + \frac{(2\rho)^{-L} \Gamma(1+2L)}{\Gamma(1+L-i\eta)} \sum_{r=0}^{\infty} P_r^{(\alpha,\beta)}(1-2\rho) M_r {}_3F_3 \left[\begin{matrix} 1+\alpha+\delta, & 1+\delta, & -L-i\eta; \\ 1+\delta-r, & \alpha+\beta+\delta+r+2, & -2L; \end{matrix} 2i \right] \right\} \right]. \quad \ldots \quad (4.8)$$

The formula (4.8) is valid under the same conditions as specified for eqn. (4.5).

5. Conclusion

As seen from eqns. (4.5) and (4.8) the Coulomb functions $F_L(\eta, \rho)$ and $G_L(\eta, \rho)$ have been expressed in the series of Jacobi and generalized confluent hypergeometric functions for all values of L. These expansions may be used for the computation of F_L and G_L for both small and large values of η, that is for both high and low energies.

In section 2, we have evaluated an integral which involves a product of Kampé de Fériet function and Jacobi polynomial. With the help of this integral an expansion formula for Kampé de Fériet function has been derived in Section 3. This expansion is of a very general nature and in turn can be transformed to generalized hypergeometric function, the product of two generalized hypergeometric functions and most of the commonly used functions in two arguments like Appell functions F_1, F_2, F_3 and F_4. Thus the results evaluated by us find application not only in the derivation of Coulomb functions but are also useful in obtaining many new results involving the generalized hypergeometric functions and the Appell's functions.

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