A Note on the Generating Function for the Coulomb Wave Functions

By

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Abstract

An attempt is made to find a generating function for the radial wave functions in the quantum mechanical Kepler problem. It is shown that for the Mellin-transformed Coulomb wave functions with a fixed angular momentum, a generating function can be represented as a double integral form. The s-wave case is studied in more detail. The generating function is simplified to a single integral form, by which the orthogonality property of the original functions is reduced to that of a new series of functions. The properties of these functions are briefly discussed.

1. Introduction

Among various two-body bound state problems in quantum mechanics, the hydrogen-like atom (Kepler problem) and the harmonic oscillator have distinguished features. They admit exact solutions and exhibit dynamical symmetries, although these facts are closely connected with each other. The analytical as well as group theoretical properties of the wave functions have been extensively studied thus far.

The (three-dimensional isotropic) harmonic oscillator problem can be solved both in the rectangular coordinates system and in the spherical polar coordinates system. The wave functions are expressed in terms of the Hermite polynomials and the Laguerre polynomials, respectively. Analogously, the hydrogen-like atom can be treated in the spherical polar coordinates system and in the parabolic coordinates system. In both cases, the wave functions are represented by the Laguerre polynomials.

From the viewpoint of the special function theory, however, there exists a significant difference between these two problems. In the harmonic oscillator

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case, the quantum numbers (principal, angular momentum, etc.) appear merely as indices of the special functions. In the hydrogen-like case, the principal quantum number appears in the argument of the special polynomials and their weight functions as a scale factor as well as in the indices. This makes it difficult in the latter case, in contrast to the former case, to find generating functions for the series of the Coulomb wave functions with different principal quantum numbers.

In this note, an attempt is made to find a generating function for the radial Coulomb wave functions with a fixed angular momentum l (the principal quantum number n takes the values $l+1$, $l+2$, ……). In the next section, the Mellin transformation is applied to the Coulomb wave functions and the generating functions for these transformed functions are obtained in a closed form. They are represented as a double integral form. The s-wave case is further elaborated in Sec. 3. The generating function is expressed as a single integral form, by which the orthonormality property of the original wave functions is reduced to the orthogonality property of a new series of functions. The properties of these new special functions are briefly discussed. The final section is devoted to a summary and discussions.

2. Mellin Transformation and Generating Functions

As is well known[1], the radial part of the normalized Coulomb wave function R_{nl}, with the principal quantum number n and the angular momentum quantum number l, is given by

$$R_{nl}(r)=-\left\{\left(\frac{2Z}{na_0}\right)^3\frac{(n-l-1)!}{2n[(n+l)!]^3}\right\}^{1/2}\exp(-r_n/2)r_n{}^l L_{n+1}^{2l+1}(r_n), \tag{1}$$
$$(l=0,1,\cdots\cdots;\ n=l+1,\ l+2,\cdots\cdots)$$

where

$$a_0=\frac{\hbar}{\mu e^2},\quad r_n=\frac{2Z}{na_0}r,\quad Z\text{; a positive integer}$$

and the Laguerre polynomial L_{n+1}^{2l+1} is defined as

$$L_{n+1}^{2l+1}(\rho)=\sum_{k=0}^{n-l-1}(-1)^{k+2l+1}\frac{[(n+l)!]^2\rho^k}{(n-l-1-k)!(2l+1+k)!k!}\,. \tag{2}$$

In order to elimate a trivial factor, we shall introduce

$$f_{nl}(r)\equiv\sum_{k=0}^{n-l-1}(-1)^k\frac{r_n{}^{l+k}}{(n-l-1-k)!(2l+1+k)!k!}\exp(-r_n/2), \tag{3}$$

so that R_{nl} is expressed in terms of f_{nl} as

$$R_{nl}(r)=\frac{2}{n^2}[(n-l-1)!(n+l)!]^{1/2}\left(\frac{Z}{a_0}\right)^{3/2}f_{nl}(r). \tag{4}$$

Since the scale-transformed variable r_n appears in Eq. (3), it is convenient to introduce the Mellin transformation to "diagonalize" the scale transformation: The Mellin transform F_{nl} of f_{nl} is defined by

$$F_{nl}(s)\equiv\int_0^\infty f_{nl}(r)r^{s-1}dr,\quad s=\sigma+i\tau. \tag{5}$$

This is well defined for σ, the real part of s, greater than $-l$. The isometric character of the transformation implies

$$\int_0^\infty f_{nl}(r)^*f_{n'l'}(r)r^{2\sigma-1}dr=\frac{1}{2\pi}\int_{-\infty}^\infty F_{nl}(\sigma+i\tau)^*F_{n'l'}(\sigma+i\tau)d\tau, \tag{6}$$

so that the orthogonality relation of $R_{nl}(r)$ with respect to the measure r^2dr is equivalent to that of $F_{nl}(3/2+i\tau)$ with respect to $d\tau$. The Mellin transform F_{nl} is calculated to be

$$F_{nl}(s)=\left(\frac{n}{2\alpha}\right)^s\sum_{k=0}^{n-l-1}(-1)^k\frac{2^{l+k+s}\Gamma(l+k+s)}{(n-l-1)!(2l+1+k)!k!}\quad\left(\alpha\equiv\frac{Z}{a_0}\right).$$

This can be rewritten, for $-l<Re(s)<l+2$, as

$$F_{nl}(s)=\left(\frac{n}{\alpha}\right)^s\frac{2^l}{(n-l-1)!\Gamma(l+2-s)}\int_0^1(t(1-t))^l\left(\frac{t}{1-t}\right)^{s-1}(1-2t)^{n-l-1}dt, \tag{7}$$

which is readily verified via a binomial expansion of $(1-2t)^{n-l-1}$.

Now, we shall derive the generating function for F_{nl} with fixed l and $n=l+1$, $l+2$, ……. By noticing that[2], for $|z|<1$,

$$\sum_{n=l+1}^\infty n^{s-l-2}z^{n-l-1}=\frac{1}{\Gamma(l+2-s)}\int_0^\infty\frac{e^{-lu}}{e^u-z}u^{l+1-s}du,$$

we find, from Eq. (7), for $|a|<1$ that

$$\begin{aligned}&\sum_{n=l+1}^\infty\frac{(n-l-1)!}{n^{l+2}}F_{nl}(s)a^{n-l-1}\\&=\frac{\alpha^{-s}2^l}{\Gamma(l+2-s)^2}\int_0^1(t(1-t))^l\left(\frac{t}{1-t}\right)^{s-1}\left[\int_0^\infty\frac{e^{-lu}}{e^u-(1-2t)a}u^{l+1-s}du\right]dt\\&=\frac{\alpha^{-s}2^l}{\Gamma(l+2-s)^2}\int_0^\infty u^{l+1-s}e^{-lu}\left[\int_0^1(t(1-t))^l\left(\frac{t}{1-t}\right)^{s-1}\frac{dt}{e^u-(1-2t)a}\right]du.\end{aligned} \tag{8}$$

In order to see the merit of the generating functions thus obtained, we shall investigate the simplest case where $l=0$ in more detail in the next section, although the integration with respect to t can be carried out explicitly for the general value of l.

3. *S*-wave Case

We have obtained in the previous section the generating function for the Mellin-transformed Coulomb wave functions for general l. It takes a rather complicated form given by Eq. (8). For the s-wave case, however, the integration with respect to t can be performed, by transforming it to a contour integral in the complex t-plane, to yield a simple result

$$\int_0^1\left(\frac{t}{1-t}\right)^{s-1}\frac{dt}{e^u-(1-2t)a}=\frac{\pi}{\sin\pi s}\left[\left(\frac{1-e^{-u}a}{1+e^{-u}a}\right)^{s-1}-1\right]\frac{1}{2a}.$$

Therefore, the generating function for $l=0$ is given by

$$\sum_{n=1}^{\infty}\frac{(n-1)!}{n^2}F_{n0}(s)a^{n-1}=\frac{\alpha^{-s}}{\Gamma(2-s)^2}\frac{\pi}{\sin\pi s}\frac{1}{2a}\int_0^{\infty}u^{1-s}\left[\left(\frac{1-e^{-u}a}{1+e^{-u}a}\right)^{s-1}-1\right]du. \quad (9)$$

Now, we shall try to derive some information from the above equality. First of all, notice that the function

$$g(u,a)=\frac{1}{u}\frac{1-e^{-u}a}{1+e^{-u}a},$$

decreases monotonously from plus infinity to zero, for the fixed real $a(-1<a<1)$, as u increases from zero to plus infinity. By putting $s=3/2+i\tau$, we obtain from Eq. (9), for $-1<a,\ b<1$, that

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{(n-1)!}{n^2}\frac{(m-1)!}{m^2}a^{n-1}b^{m-1}\frac{1}{2\pi}\int_{-\infty}^{\infty}F_{n0}(3/2+i\tau)^*F_{m0}(3/2+i\tau)d\tau$$
$$=\frac{\alpha^{-3}}{4ab}\int_0^{\infty}du\int_0^{\infty}dv\int_{-\infty}^{\infty}d\tau\left\{\sqrt{g(u,a)g(v,b)}\left(\frac{g(v,b)}{g(v,a)}\right)^{i\tau}\right.$$
$$-\sqrt{g(u,0)g(v,b)}\left(\frac{g(v,b)}{g(u,0)}\right)^{i\tau}-\sqrt{g(u,a)g(v,0)}\left(\frac{g(v,0)}{g(u,a)}\right)^{i\tau}$$
$$\left.+\sqrt{g(u,0)g(v,0)}\left(\frac{g(v,0)}{g(u,0)}\right)^{i\tau}\right\}=\frac{\alpha^{-3}}{4ab}\int_0^{\infty}du\int_0^{\infty}dv$$
$$\times\left\{\sqrt{g(u,a)g(v,b)}\,\delta\left(\log\frac{g(v,b)}{g(u,a)}\right)-\sqrt{g(u,0)g(v,b)}\,\delta\left(\log\frac{g(v,b)}{g(u,0)}\right)\right.$$
$$\left.-\sqrt{g(u,a)g(v,0)}\,\delta\left(\log\frac{g(v,0)}{g(u,a)}\right)+\sqrt{g(u,0)g(v,0)}\,\delta\left(\log\frac{g(v,0)}{g(u,0)}\right)\right\}. \quad (10)$$

In the above derivation we have used the well-known formula[3)]

$$\frac{1}{\Gamma(1/2-i\tau)^2\Gamma(1/2+i\tau)^2}\frac{\pi^2}{\sin\pi(3/2+i\tau)\sin\pi(3/2-i\tau)}$$
$$=\left(\frac{1}{\Gamma(1/2-i\tau)\Gamma(1/2+i\tau)}\frac{\pi}{\cos\pi i\tau}\right)^2=1.$$

Because of the equality

$$\int_0^\infty dv\sqrt{g(u,a)g(v,0)}\,\delta\Big(\log\frac{g(v,0)}{g(u,a)}\Big)=g(u,a)\int_0^\infty dv\delta(\log v+\log g(u,a))$$
$$=g(u,a)\int_0^\infty dv\,v\delta\Big(v-\frac{1}{g(u,a)}\Big)=1,$$

the right hand side of Eq. (10) can be rewritten as

$$\frac{\alpha^{-3}}{4ab}\int_0^\infty du\int_0^\infty dv\Big\{\sqrt{g(u,a)g(v,b)}\,\delta\Big(\log\frac{g(v,b)}{g(u,a)}\Big)$$
$$-\sqrt{g(u,0)g(v,0)}\,\delta\Big(\log\frac{g(v,0)}{g(u,0)}\Big)\Big\}.$$

Consequently, from Eqs. (4) and (6), we find that Eq. (10) reduces to

$$\sum_{n=1}^\infty\sum_{m=1}^\infty\frac{1}{\sqrt{nm}}a^{n-1}b^{m-1}\int_0^\infty R_{n0}(r)R_{m0}(r)r^2dr$$
$$=\frac{1}{ab}\int_0^\infty du\int_0^\infty\Big\{\sqrt{g(u,a)g(v,b)}\,\delta\Big(\log\frac{g(v,b)}{g(u,a)}\Big)$$
$$-\sqrt{g(u,0)g(v,0)}\,\delta\Big(\log\frac{g(v,0)}{g(u,0)}\Big)\Big\}\Big(\equiv\frac{1}{ab}G(a,b)\Big). \tag{11}$$

Unfortunately, the integration on the right hand side of this equation cannot be performed analytically for the general values of a and b. For the special case where $a=b$, since the equation $g(v,a)=g(u,a)$ is solved to give $v=u$, we can carry out the integration;

$$G(a,a)=\int_0^\infty du\Big\{g(u,a)\Big(\frac{g(v,a)}{|\partial g(v,a)/\partial v|}\Big)_{v=u}-1\Big\}$$
$$=\int_0^\infty du\,\frac{2(e^{-2u}a^2-e^{-u}a+ue^{-u}a)}{1-e^{-2u}a^2-2ue^{-u}a}=\Big[\log(1-e^{-2u}a^2-2ue^{-u}a)\Big]_0^\infty$$
$$=-\log(1-a^2).$$

Therefore, if it can be shown that $G(a,b)$ is a function of $a\cdot b$ only, so that its value at (a,b) is equal to that at $(\sqrt{ab},\sqrt{ab})$; $G(a,b)=G(\sqrt{ab},\sqrt{ab})=-\log(1-ab)$, then Eq. (11) becomes

$$\sum_{n=1}^\infty\sum_{m=1}^\infty\frac{1}{\sqrt{nm}}a^{n-1}b^{m-1}\int_0^\infty R_{n0}(r)R_{m0}(r)r^2dr=-\frac{1}{ab}\log(1-ab). \tag{12}$$

This is nothing but the orthonormality condition

$$\int_0^\infty R_{n0}(r)R_{m0}(r)r^2dr=\delta_{n,m}. \tag{13}$$

We shall, at this point, invert the order of our induction by admitting the orthonormality condition (13), and hence Eq. (12), and try to see the consequences of Eq. (11). By means of the inverse function of $g(u,a)$;

$$\frac{1}{x}=g(u,a)\rightleftarrows u=h(x,a),\quad -1<a<1\ (0<x,\ u<\infty),$$

Eq. (11) is transformed into

$$\begin{aligned}G(a,b)=&\int_{-\infty}^{\infty}d(\log x)\int_0^{\infty}du\int_0^{\infty}dv\,\{\sqrt{g(u,a)g(v,b)}\,\delta(\log g(u,a)+\log x)\\&\times\delta(\log g(v,b)+\log x)-\sqrt{g(u,0)g(v,0)}\,\delta(\log g(u,0)+\log x)\\&\times\delta(\log g(v,0)+\log x)\}\\=&\int_0^{\infty}\frac{dx}{x^2}\left\{\int_0^{\infty}du\,\delta(\log g(u,a)+\log x)\int_0^{\infty}dv\,\delta(\log g(v,b)+\log x)\right.\\&\left.-\int_0^{\infty}du\,\delta(\log u-\log x)\int_0^{\infty}dv\,\delta(\log v-\log x)\right\}\\=&\int_0^{\infty}\frac{dx}{x^2}\left\{\int_0^{\infty}du\,\delta(u-h(x,a))\frac{g(u,a)}{|\partial g(u,a)/\partial u|}\int_0^{\infty}dv\,\delta(v-h(x,b))\right.\\&\left.\times\frac{g(v,b)}{|\partial g(v,a)/\partial v|}-x^2\right\}=\int_0^{\infty}dx\left\{\frac{\partial}{\partial x}h(x,a)\frac{\partial}{\partial x}h(x,b)-1\right\},\end{aligned}\tag{14}$$

where use has been made of the equality

$$\left.\frac{g(u,a)}{|\partial g(u,a)/\partial u|}\right|_{u=h(x,a)}=\frac{1}{x}\cdot x^2h(x,a).$$

The equality $G(a,b)=-\log(1-ab)$, therefore, implies

$$\int_0^{\infty}dx\left\{\frac{\partial}{\partial x}h(x,a)\frac{\partial}{\partial x}h(x,b)-1\right\}=-\log(1-ab).\tag{15}$$

Obviously, for the fixed x in $0<x<\infty$, the function $\partial h(x,a)/\partial x$ is a real analytic function of a in the region $-1<a<1$. As a consequence, the power series expansion is allowed as follows

$$\frac{\partial}{\partial x}h(x,a)=\sum_{k=0}^{\infty}X_k(x)a^k.\tag{16}$$

Thus, as is seen from Eq. (15), we have obtained a new series of orthogonal functions $X_k(x)$;

$$\int_0^{\infty}X_j(x)X_k(x)dx=0\qquad\text{for } j\neq k,\tag{17}$$

with the norm property

$$\int_0^{\infty}(X_k(x))^2dx=\frac{1}{k}\qquad\text{for } k=1,2,\cdots\cdots.\tag{18}$$

The first few terms of X_k are

$$X_0(x)=1,\quad X_1(x)=2(x-1)e^{-x},\quad X_2(x)=2(4x^2-6x+1)e^{-2x}.$$

In general, X_k is shown to be of the form $X_k(x)=p_k(x)\cdot e^{-kx}$, where p_k is a polynomial of order k. Remembering that $R_{n0}(r)$ is of the form (n-th order polynomial of r) $\times e^{-r/n}$, we can regard X_k to be "dual" to the original Coulomb wave functions. The weight of $X_k(x)$, i.e. e^{-kx}, depends on k analogously as in the case of R_{n0}. We have, however, a good reason to believe that the new series of special functions is more tractable than the original ones. For, if we could find a generating function for the polynomial part p_k;

$$P(x, a)=\sum_{k=0}^{\infty} c_k p_k(x) a^k,$$

then the generating function for X_k would immediately follow:

$$P(x, e^{-x}a)=\sum_{k=0}^{\infty} c_k X_k(x) a^k.$$

4. Summary and Discussion

We have found the generating functions for the Mellin-transformed Coulomb wave functions. For the general value of the angular momenta, they are given by Eq. (8), and for the s-wave case, by Eq. (9). Instead of proving the orthonormality property (13), we have reversed the direction of our induction. From Eq. (12), it is shown that the new series of functions defined by Eq. (16) satisfies the orthonormality relation (17) and (18). Thus, there naturally arises the new series of orthogonal functions in association with the Coulomb wave functions. Since the Coulomb wave functions have a definite group theoretical meaning, it is hopeful to develop the group theoretical argument concerning the property of these special functions in the sense of Vilenkin's textbook[4]. Also, it is highly desirable to find another generating function which enables an explicit calculation of the general form of the series, although we have one defined by an implicit function, Eq. (16).

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