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An Alternative Approach to Calculating the Mean Values $\overline{r^k}$ for Hydrogen-Like Atoms

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Abstract

Based on the exact expressions of the integral for two confluent hypergeometric functions systematically obtained by the MATHEMATICA package INTEPFFLL, we obtain the mean values $\overline{r^k}(|k| \leq 8)$ for hydrogen-like atoms analytically. It is found that these formulas are very useful in quantum mechanics and atomic physics.

1. Introduction

It is well known that the exact solutions of the Schrödinger equation with central physical potentials have been the subject of interest in quantum mechanics. For example, the exact solutions of the Schrödinger equation for a hydrogen atom in three dimensions [1,2] were important achievements at the beginning stage of quantum mechanics, which provided a strong evidence in favor of the theory being correct. To obtain the exact solutions of some quantum systems, we will calculate the normalization factor since it plays an important role in constructing ladder operators as shown in our recent work [3–11]. Generally speaking, the exact solutions of some quantum systems can be expressed by the confluent hypergeometric functions or by the associated Laguerre functions. Hence, the calculation of the normalization factor and matrix elements for some physical functions becomes the calculation of the integral of two confluent hypergeometric functions or two associated Laguerre functions multiplied by a factor $e^{-\rho}\rho^{\nu}(\nu > -1)$.

The purpose of this work is two-fold. The first is to systematically obtain the exact expressions of the integral for two confluent hypergeometric functions or two associated Laguerre functions in terms of the MATHEMATICA package INTEPFFLL programmed by Qiang [12]. These exact expressions are very useful in quantum mechanics and atomic physics. The second, which is the main purpose of this work, is to make use of the exact expressions and the MATHEMATICA package INTEPFFLL to obtain the mean value $\overline{r^k}(|k| \leq 8)$, which is needed for the multipole corrections in calculation on atomic spectral terms. The calculations for $k = -5, -6$ were discussed by Van Vleck [13] in terms of the Fourier series expansion method seventy years ago, but the expressions of those mean values were not explicit and very complicated. Also there existed a typo[1] for the mean value $\overline{r^{-6}}$. Since then, the derivations of the mean values $\overline{r^k}(|k| \leq 4)$ have been investigated in Refs. [2,14,15].

This paper is organized as follows. In Section 2 we derive some exact expressions of the integral for two confluent hypergeometric functions or two associated Laguerre functions multiplied by a factor $e^{-\rho}\rho^{\nu}(\nu > -1)$. Section 3 is devoted to the calculation of the mean values $\overline{r^k}(|k| \leq 8)$. Concluding remarks are given in Section 4.

2. The derivation of the integral formula

To our knowledge, a number of formulas to calculate the integral for two confluent hypergeometric functions have appeared [2,14–20],

$$J(\alpha, \gamma, \alpha', \gamma', \rho) = \int_0^\infty e^{-\rho}\rho^{\nu}\, {}_1F_1(\alpha, \gamma, \rho)\, {}_1F_1(\alpha', \gamma', \rho)\, d\rho, \quad \nu > -1, \tag{1}$$

where ${}_1F_1(\alpha, \gamma, \rho)$ and ${}_1F_1(\alpha', \gamma', \rho)$ are confluent hypergeometric functions. α and α' are negative integers or zeros. Generally speaking, the well-known formulas are limited to some special cases, e.g., the formulas given in [21] are only useful in numerical calculations. To obtain the normalization factor and matrix element for some physical functions such as the mean values $\overline{r^k}$, it is necessary to derive exact expressions of the integral for two confluent hypergeometric functions or two associated Laguerre functions. For simplicity, we study only the following integrals

$$I_{LL}(n, \triangle n, \beta, \triangle\beta, \lambda) = \int_0^\infty e^{-\rho}\rho^{\beta+\lambda} L_n^{\beta}(\rho) L_{n+\triangle n}^{\beta+\triangle\beta}(\rho)\, d\rho, \tag{2}$$

and

$$I_{FF}(n, \triangle n, \beta, \triangle\beta, \lambda) = \int_0^\infty e^{-\rho}\rho^{\beta+\lambda}\, {}_1F_1(-n, \beta, \rho)\, {}_1F_1(-n - \triangle n, \beta + \triangle\beta, \rho)\, d\rho, \tag{3}$$

where $\triangle n \geq 0$ and $\triangle n, \triangle\beta, \lambda$ are integers. We assume that n is a non-negative integer, and $\beta, \beta + \triangle\beta$ are not equal to zero or negative integers.

[1]The numerical form of $\overline{r^{-6}} \times a_0^6/Z^6$ written by $0.06173n^{-3} - 0.27336n^{-5} + 0.12698n^{-7}$ should be corrected as $0.006173n^{-3} - 0.027336n^{-5} + 0.012698n^{-7}$.

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We first consider integral (2). This integral can be further expressed as [20]

$$\int_0^\infty e^{-\rho}\rho^{\beta+\lambda}L_n^\beta(\rho)L_{n+\Delta n}^{\beta+\Delta\beta}(\rho)\,d\rho = (-1)^{\Delta n}\Gamma(1+\beta+\lambda) \times \sum_k \binom{\lambda}{n-k}\binom{\lambda-\Delta\beta}{n+\Delta n-k}\binom{\beta+\lambda+k}{k}. \tag{4}$$

It is found that $k_{\max} = n$, but $k_{\min} \geq 0$, i.e.,

$$k_{\min} = \begin{cases} 0, & \text{for } \lambda < 0 \text{ and } \lambda - \Delta\beta < 0; \\ \mathrm{Min}(n, n+\Delta n - \lambda + \Delta\beta), & \text{for } \lambda < 0 \text{ and } \lambda - \Delta\beta \geq 0; \\ \mathrm{Min}(n, n-\lambda), & \text{for } \lambda \geq 0 \text{ and } \lambda - \Delta\beta < 0; \\ n, & \text{for } \lambda \geq 0 \text{ and } \lambda - \Delta\beta \geq 0 \text{ and } \mathrm{Max}(n-\lambda, n+\Delta n-\lambda+\Delta\beta) \geq n; \\ \mathrm{Max}(n-\lambda, n+\Delta n - \lambda + \Delta\beta), & \text{for } \lambda \geq 0 \text{ and } \lambda - \Delta\beta \geq 0 \text{ and } \mathrm{Max}(n-\lambda, n+\Delta n-\lambda+\Delta\beta) < n. \end{cases} \tag{5}$$

where we have assumed that $\mathrm{Max}(n-\lambda, n+\Delta n-\lambda+\Delta\beta) \geq 0$. For given Δn, $\Delta\beta$ and λ, we can obtain various closed expressions of integral (2).

Let us consider integral (3). Using the relation between the associated Laguerre polynomials and the confluent hypergeometric functions as [18,20]

$$L_n^\mu(\rho) = \frac{\Gamma(\mu+1+n)}{n!\Gamma(\mu+1)}\,{}_1F_1(-n, \mu+1, \rho), \tag{6}$$

we can reexpress Eq. (3) as

$$\begin{aligned} I_{FF}(n, \Delta n, \beta, \Delta\beta, \lambda) &= \int_0^\infty e^{-\rho}\rho^{\beta+\lambda}\,{}_1F_1(-n, \beta, \rho) \times {}_1F_1(-(n+\Delta n), \beta+\Delta\beta, \rho)\,d\rho \\ &= \frac{n!(n+\Delta n)!\Gamma(\beta)\Gamma(\beta+\Delta\beta)}{\Gamma(n+\beta)\Gamma(n+\Delta n+\beta+\Delta\beta)} \times I_{LL}(n, \Delta n, \beta-1, \Delta\beta, \lambda+1). \end{aligned} \tag{7}$$

For given $\Delta n, \Delta\beta$ and λ, we can obtain closed expressions of Eq. (3). For simplicity, some formulas given in Table I (see Appendix I) are used to calculate the mean values $\overline{r^k}$.

3. The mean values $\overline{r^k}$ for hydrogen-like atoms

Before proceeding, we derive the normalization factor using the results given in Table I. For a Coulomb field $V = -\xi/r$ with $\xi = Z\alpha$ ($\alpha \simeq 1/137$), from the Coulomb units the exact solutions of the radial Schrödinger equation are given by [2]

$$R_{nl} = N_{nl}(2r)^l e^{-r/n}\,{}_1F_1(-n+l+1, 2l+2, 2r/n), \tag{8}$$

where n and l are principal quantum number and angular momentum quantum number, respectively. N_{nl} is the normalization constant to be determined by the normalization condition

$$\begin{aligned} \int_0^\infty R_{nl}(r)^2 r^2\,dr &= \int_0^\infty N_{nl}^2 2^{2l} r^{2l+2} e^{-2r/n} \times {}_1F_1(-n+l+1, 2l+2, 2r/n)^2\,dr \\ &= N_{nl}^2\left(\frac{n}{2}\right)^{2l+3} 2^{2l} I_{FF}(n-l-1, 0, 2l+2, 0, 0) \\ &= 1, \end{aligned} \tag{9}$$

which implies that $\Delta n = 0$, $\Delta\beta = 0$ and $\lambda = 0$. From Table I, it is easy to obtain [2]

$$N_{nl} = \frac{2}{n^{l+2}(2l+1)!}\sqrt{\frac{(n+l)!}{(n-l-1)!}}. \tag{10}$$

Because of its importance in quantum mechanics and atomic physics, we now make use of the MATHEMATICA package INTEPFFLL to derive the mean values $\overline{r^k}$ systematically in the background of the Coulomb field. $\overline{r^k}$ can be expressed as

$$\begin{aligned} \overline{r^k} &= \int_0^\infty R_{nl}(r)^2 r^{2+k} dr \\ &= \int_0^\infty N_{nl}^2 2^{2l} r^{2l+2+k} e^{-2r/n}\,{}_1F_1(-n+l+1, 2l+2, 2r/n)^2\,dr \\ &= N_{nl}^2\left(\frac{n}{2}\right)^{2l+3+k} 2^{2l} I_{FF}(n-l-1, 0, 2l+2, 0, k). \end{aligned} \tag{11}$$

Using the results of $I_{FF}(n, 0, \beta, 0, k)$ obtained by the MATHEMATICA package INTEPFFLL, we can easily obtain the mean values $\overline{r^k}$ ($|k| \leq 4$) as

$$\bar{r} = \tfrac{1}{2}[3n^2 - l(l+1)], \tag{12a}$$

$$\overline{r^2} = \frac{n^2}{2}[5n^2 + 1 - 3l(l+1)], \tag{12b}$$

$$\overline{r^3} = \frac{n^2}{8}\{3(l-1)l(l+1)(l+2) - 5[6l(l+1) - 5]\,n^2 + 35\,n^4\}, \tag{12c}$$

$$\overline{r^4} = \frac{n^4}{8}\{5l(l+1)[3l(l+1)-10] - 70l(l+1)n^2 + 63n^4 + 3(4+35n^2)\}, \tag{12d}$$

and

$$\overline{r^{-1}} = \frac{1}{n^2}, \tag{13a}$$

$$\overline{r^{-2}} = \frac{1}{n^3(l+1/2)}, \tag{13b}$$

$$\overline{r^{-3}} = \frac{2}{l(1+l)(1+2l)n^3}, \tag{13c}$$

$$\overline{r^{-4}} = -\frac{4(l+l^2-3n^2)}{l(1+l)(-1+2l)(1+2l)(3+2l)n^5}. \tag{13d}$$

It is found that these results coincide with those given in [2,15].

With increasing $|k|$, the expressions for the mean values $\overline{r^k}$ ($|k| \geq 5$) are more complicated. Nevertheless, due to their possible applications in atomic physics[2], the mean values $\overline{r^{-5}}$ and $\overline{r^{-6}}$ were given by Van Vleck [13], but the expressions given by him were not expressed explicitly by parameters n and l. For this purpose, making use of the MATHEMATICA package INTEPFFLL, we obtain exactly explicit expressions for the mean values $\overline{r^k}$ ($|k| \in [5,8]$) which are sometimes useful,

$$\overline{r^5} = \frac{n^4}{16}\{-5(l-2)(l-1)l(l+1)(l+2)(l+3) + 21[14+5l(1+l)(l^2+l-5)]n^2 - 105[3l(l+1)-7]n^4 + 231n^6\}, \tag{14a}$$

$$\overline{r^6} = \frac{n^6}{16}\{180 - 7l(l+1)[126+5l(l+1)(l^2+l-11)] + [2121+315l(l+1)(l^2+l-7)]n^2 - 231[3l(l+1)-10]n^4 + 429n^6\}, \tag{14b}$$

$$\overline{r^7} = \frac{n^6\,\Gamma(n-l)}{256(n+l)!}\left[\frac{(n+l)!}{\Gamma(-8-l+n)} + \frac{64(7+l+n)!}{\Gamma(-1-l+n)} + \frac{64\Gamma(2+l+n)}{\Gamma(-7-l+n)} + \frac{784\Gamma(3+l+n)}{\Gamma(-6-l+n)}. + \frac{3136\Gamma(4+l+n)}{\Gamma(-5-l+n)} + \frac{4900\Gamma(5+l+n)}{\Gamma(-4-l+n)} + \frac{3136\Gamma(6+l+n)}{\Gamma(-3-l+n)} + \frac{784\Gamma(7+l+n)}{\Gamma(-2-l+n)} + \frac{\Gamma(9+l+n)}{\Gamma(-l+n)}\right], \tag{14c}$$

$$\overline{r^8} = \frac{n^7\Gamma(-l+n)}{512(l+n)!}\left[\frac{(l+n)!}{\Gamma(-9-l+n)} + \frac{1296(7+l+n)!}{\Gamma(-2-l+n)} + \frac{81\Gamma(2+l+n)}{\Gamma(-8-l+n)} + \frac{1296\Gamma(3+l+n)}{\Gamma(-7-l+n)} + \frac{7056\Gamma(4+l+n)}{\Gamma(-6-l+n)} + \frac{15876\Gamma(5+l+n)}{\Gamma(-5-l+n)} + \frac{15876\Gamma(6+l+n)}{\Gamma(-4-l+n)} + \frac{7056\Gamma(7+l+n)}{\Gamma(-3-l+n)} + \frac{81\Gamma(9+l+n)}{\Gamma(-1-l+n)} + \frac{\Gamma(10+l+n)}{\Gamma(-l+n)}\right], \tag{14d}$$

and

$$\overline{r^{-5}} = -\frac{4\left[3l(l+1)-1-5n^2\right]}{(l-1)l(l+1)(l+2)(2l-1)(2l+1)(2l+3)n^5}, \tag{15a}$$

$$\overline{r^{-6}} = \frac{4\{3(l-1)l(l+1)(l+2) - 5[6l(l+1)-5]n^2 + 35n^4\}}{(l-1)l(l+1)(l+2)(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)n^7}, \tag{15b}$$

$$\overline{r^{-7}} = \frac{4}{(l-2)_6} \times \frac{12 + 5l(l+1)[3l(l+1)-10] + [105-70l(l+1)]n^2 + 63n^4}{(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)n^7}, \tag{15c}$$

$$\overline{r^{-8}} = -\frac{8}{(l-2)_6} \times 5(-2+l)_6 - 21[14+5l(l+1)(l^2+l-5)]n^2 \frac{+105[3l(l+1)-7]n^4 - 231n^6}{(2l-5)(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)(2l+7)n^9}, \tag{15d}$$

where $(\alpha)_n$ stands for Pochhammer symbol [17]. For any k, we can, in principle, obtain all mean values $\overline{r^k}$ with the MATHEMATICA package INTEPFFLL [12]. Nevertheless, with increasing $|k|$, the calculations of the mean values $\overline{r^k}$($|k| \geq 9$) become more complicated.

4. Concluding remarks

Making use of exact expressions of the integral for two confluent hypergeometric functions or two associated Laguerre functions obtained by the MATHEMATICA package INTEPFFLL, we have systematically obtained analytical expressions of the mean values $\overline{r^k}$($|k| \leq 8$). It is found that these results are very useful in quantum mechanics since many exact solutions of quantum systems with certain central physical potentials could be expressed by confluent hypergeometric functions or associated Laguerre functions. For example, these results have been applied to calculate the normalization factor of the harmonic oscillator [22]. It should be pointed out that we can use this MATHEMATICA package INTEPFFLL [12] to automatically obtain $I_{FF}(n, \Delta n, \beta, \Delta\beta, \lambda)$ and

[2]For example, the mean value $\overline{r^{-6}}$ is needed for the quadrupole corrections in calculations on atomic spectral terms.

$I_{LL}(n, \Delta n, \beta, \Delta\beta, \lambda)$. Further, we can apply these results to derive the normalization factor for the Dirac equation with the Coulomb potential [23].

Appendix I Some exact expressions of the integrals

In this Appendix, we give some exact expressions of the integral for two confluent hypergeometric functions in terms of the MATHEMATICA package INTEPFFLL.

Table I: *Some exact expressions of the integral (3).*

λ	Δn	$\Delta\beta$	I_{FF}
1	1	1	$-\frac{(1+n)!\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(n+\beta)}$
0	0	0	$\frac{(2n+\beta)n!\Gamma(\beta)^2}{\Gamma(n+\beta)}$
1	1	0	$-\frac{2(1+2n+\beta)(1+n)!\Gamma(\beta)^2}{\Gamma(n+\beta)}$
1	0	1	$\frac{(1+3n+\beta)n!\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(n+\beta)}$
0	1	1	0
1	0	0	$\frac{(6n^2+\beta+6n\beta+\beta^2)n!\Gamma(\beta)^2}{\Gamma(n+\beta)}$
0	0	1	$\frac{n!\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(n+\beta)}$
0	1	0	$-\frac{(1+n)!\Gamma(\beta)^2}{\Gamma(n+\beta)}$
−1	1	0	0
1	0	−1	$\frac{[2n(-1+5n)+\beta+8n\beta+\beta^2]n!\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(-1+n+\beta)}$
−1	0	1	$\frac{n!\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(1+n+\beta)}$
0	1	−1	$-\frac{(3n+2\beta)(1+n)!\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(n+\beta)}$
−1	0	0	$\frac{n!\Gamma(\beta)^2}{\Gamma(n+\beta)}$
0	0	−1	$\frac{n!(3n+\beta)\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(-1+n+\beta)}$
1	1	−1	$-\frac{[10n^2+3\beta(1+\beta)+2n(1+6\beta)](1+n)!\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(n+\beta)}$
−1	1	1	$\frac{(1+n)!\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(2+n+\beta)}$
−1	1	−1	$-\frac{(1+n)!\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(n+\beta)}$
−1	0	−1	$\frac{n!\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(-1+n+\beta)}$

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