A Note on the Wave Functions of the Relativistic Hydrogenic Atom

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The radial functions for the discrete levels of Dirac's relativistic hydrogenic atom are expressed in terms of the generalized Laguerre polynomials which have known properties. This leads to an easy method of evaluating the normalization constants and the average values of r^q.

IT DOES not appear to have been noticed that the radial functions that arise in the treatment of Dirac's relativistic hydrogenic atom can be expressed in terms of generalized Laguerre polynomials. The ease of handling the radial functions for the discrete levels is greatly increased if use is made of the known properties[1] of these polynomials.

The generalized Laguerre polynomial, $\mathfrak{L}_n^{(\alpha)}(z)$, is defined in terms of the confluent hypergeometric function[2] as

$$\mathfrak{L}_n^{(\alpha)}(z)=\Gamma(\alpha+n+1)/[n!\Gamma(\alpha+1)] \times {}_1F_1(-n;\alpha+1;z), \quad (1)$$

where n is a non-negative integer and α may be any complex number. It should be noted that the generalized Laguerre polynomial, $\mathfrak{L}_n^{(\alpha)}(z)$, is not the same as the ordinary[3] associated Laguerre polynomial, $L_n^m(z)$. The relation between them is

$$\mathfrak{L}_n^{(m)}(z)=(-1)^m[(n+m)!]^{-1}L_{n+m}^m(z),$$

if m is a non-negative integer. It seems to be more convenient to introduce the mathematicians' generalized Laguerre polynomial, $\mathfrak{L}_n^{(\alpha)}$, than to generalize the physicists' associated Laguerre polynomial, L_n^m, in such a way that it is defined for a non-integral superscript. The subscript, n, indicates the degree of the polynomial $\mathfrak{L}_n^{(\alpha)}$, while the degree of L_β^α, if generalized, would be $\beta-\alpha$, where neither α nor β are integers, in general.

We shall take as the radial functions of the relativistic hydrogenic atom those given by Hill and Landshoff.[4] They are $f(r)$, $G(r)$, $F(r)$, and $g(r)$. By letting either the first two or the last two vanish identically, we get two independent solutions. We can secure greater conciseness by introducing a parameter, s, that can take on either of the two values $+1$ or -1. We then define the functions $f_s(r)$ and $G_s(r)$ by the equations

$$f_s(r)=\begin{cases} f(r) & \text{when } s=+1 \\ F(r) & \text{when } s=-1, \end{cases}$$
$$G_s(r)=\begin{cases} G(r) & \text{when } s=+1 \\ g(r) & \text{when } s=-1. \end{cases}$$

Using Hill and Landshoff's Eqs. (82)–(99), we have

$$\alpha=e^2/\hbar c, \quad \lambda=(m_0c/\hbar)(1-\epsilon^2)^{\frac{1}{2}}, \quad \rho=2\lambda r,$$
$$\epsilon=E/m_0c^2=[1+Z^2\alpha^2/(n'+\gamma)^2]^{-\frac{1}{2}},$$
$$\gamma=[(J+\tfrac{1}{2})^2-Z^2\alpha^2]^{\frac{1}{2}}, \quad (2)$$

where the electronic charge is e, the energy is E, and the rest mass of the electron is m_0. In terms of these abbreviations we find that

$$f_s(r)=isC(1-s\epsilon)^{\frac{1}{2}}(e^{-\lambda r}/r)\rho^\gamma(v_{1,s}-v_{2,s}),$$
$$G_s(r)=C(1+s\epsilon)^{\frac{1}{2}}(e^{-\lambda r}/r)\rho^\gamma(v_{1,s}+v_{2,s}), \quad (3)$$

where

$$v_{1,s}=(2\gamma+n')[\gamma+n'+s(J+\tfrac{1}{2})\epsilon]^{-\frac{1}{2}}\epsilon\mathfrak{L}_{n'-1}^{(2\gamma)}(\rho),$$
$$v_{2,s}=-s[\gamma+n'+s(J+\tfrac{1}{2})\epsilon]^{\frac{1}{2}}\mathfrak{L}_{n'}^{(2\gamma)}(\rho), \quad (4)$$
$$C=\lambda(n'!\hbar)^{\frac{1}{2}}[2Z\alpha m_0c\epsilon\Gamma(2\gamma+n'+1)]^{-\frac{1}{2}}.$$

Our quantum numbers, n' and J, are connected with the usual quantum numbers, n and l, of the nonrelativistic theory by the equations

$$n=n'+J+\tfrac{1}{2}, \quad l=J-\tfrac{1}{2}s.$$

[1] E. T. Copson, *Functions of a Complex Variable* (Oxford University Press, 1935), pp. 269–270. G. Pólya and G. Szegö, *Aufgaben und Lehrsätze aus der Analysis*, Vol. 2 (Springer, 1925), p. 293.
[2] E. T. Copson, reference 1, p. 290.
[3] H. Bethe, *Handbuch der Physik*, second edition, Vol. 24 (1933), p. 282.
[4] E. L. Hill and R. Landshoff, Rev. Mod. Phys. **10**, 87, 107–110 (1938).

The evaluation of the normalization factor, C, is readily carried out. In accordance with Hill and Landshoff's Eq. (D1), we see that we must have

$$1=\int_0^\infty |rf_s|^2dr+\int_0^\infty |rG_s|^2dr.$$

If we use the equation

$$\int_0^\infty e^{-x}x^\alpha \mathfrak{L}_m^{(\alpha)}(x)\mathfrak{L}_n^{(\alpha)}(x)dx =\begin{cases}0 & \text{if } m\neq n\\ \Gamma(\alpha+n+1)/n! & \text{if } m=n,\end{cases}$$

the integral converging if $R(\alpha)>-1$, elementary algebra gives the expression for C found above.

In order to calculate the average value of r^q, we must first evaluate the integral[5]

$$I_{m,\,n}^{(\alpha)}(q)=\int_0^\infty e^{-x}x^{\alpha+q}\mathfrak{L}_m^{(\alpha)}(x)\mathfrak{L}_n^{(\alpha)}(x)dx, \quad (5)$$

where $m<n$. The generating function for the generalized Laguerre polynomials is

$$(1-t)^{-\alpha-1}e^{-xt/(1-t)}=\sum_{n=0}^\infty t^n\mathfrak{L}_n^{(\alpha)}(x), \quad |t|<1.$$

We multiply this by a similar equation in which t^n is replaced by u^m. If we then multiply by $e^{-x}x^{\alpha+q}$ and integrate, we can derive the equation

$$I_{m,\,n}^{(\alpha)}(q)=(-q)_{n-m}\Gamma(\alpha+q+m+1) \times[(n-m)!m!]^{-1}\,{}_3F_2\begin{bmatrix}-q, & -q+n-m, & -m\\ n-m+1, & -\alpha-q-m\end{bmatrix}. \quad (6)$$

The integral does not converge unless $R(\alpha+q+1)>0$ and is zero if q is an integer such that $0\leqslant q<n-m$. $(-q)_{n-m}$ is either $\Gamma(-q+n-m)/\Gamma(-q)$ or $(-1)^{n-m}\Gamma(q+1)/\Gamma(q-n+m+1)$, whichever has meaning. ${}_3F_2$ is the generalized hypergeometric function[6] with unit argument,

$${}_3F_2\begin{bmatrix}a, b, c\\ e, f\end{bmatrix}=1+\frac{abc}{1!ef}+\frac{a(a+1)b(b+1)c(c+1)}{2!e(e+1)f(f+1)}+\cdots.$$

We see from Hill and Landshoff that

$$\begin{aligned}\langle r^q\rangle_{\mathrm{Av}}&=\iiint\psi^*r^q\psi dxdydz\\ &=\int_0^\infty r^q(|rf_s|^2+|rG_s|^2)dr\\ &=2C^2(2\lambda)^{-q-1}\{(2\gamma+n')^2\epsilon^2\\ &\quad\times[\gamma+n'+s(J+\tfrac{1}{2})\epsilon]^{-1}I_{n'-1,\,n'-1}^{(2\gamma)}(q)\\ &\quad-2\epsilon^2(2\gamma+n')I_{n'-1,\,n'}^{(2\gamma)}(q)\\ &\quad+[\gamma+n'+s(J+\tfrac{1}{2})\epsilon]\dot{I}_{n',\,n'}^{(2\gamma)}(q)\}\\ &=\frac{\hbar\lambda}{2Z\alpha m_0c\epsilon}\left(\frac{1}{2\lambda}\right)^q\frac{\Gamma(2\gamma+q+n')}{\Gamma(2\gamma+n'+1)}\\ &\quad\times\left\{\frac{n'(2\gamma+n')^2\epsilon^2}{\gamma+n'+s(J+\frac{1}{2})\epsilon}\right.\\ &\quad\times{}_3F_2\begin{bmatrix}-q, & -q, & -n'+1\\ 1, & -2\gamma-q-n'+1\end{bmatrix}\\ &\quad+2n'\epsilon^2q(2\gamma+n')\\ &\quad\times{}_3F_2\begin{bmatrix}-q, & -q+1, & -n'+1\\ 2, & -2\gamma-q-n'+1\end{bmatrix}\\ &\quad+[\gamma+n'+s(J+\tfrac{1}{2})\epsilon](2\gamma+q+n')\\ &\quad\left.\times{}_3F_2\begin{bmatrix}-q, & -q, & -n'\\ 1, & -2\gamma-q-n'\end{bmatrix}\right\}. \quad (7)\end{aligned}$$

In case q is negative, it is often convenient to use the equation[7]

$$\begin{aligned}&{}_3F_2\begin{bmatrix}-q, & -q+n-m, & -m\\ n-m+1, & -\alpha-q-m\end{bmatrix}\\ &=\frac{\Gamma(\alpha+m-q)\Gamma(\alpha+q+1)}{\Gamma(\alpha-q)\Gamma(\alpha+q+m+1)}\\ &\quad\times{}_3F_2\begin{bmatrix}q+1, & q+1+n-m, & -m\\ n-m+1, & -m+q-\alpha+1\end{bmatrix}. \quad (8)\end{aligned}$$

If we let $c\rightarrow\infty$, getting the nonrelativistic approximation, Eq. (7) reduces to the expressions given by Pasternack[8] for $\langle r^q\rangle_{\mathrm{Av}}$ in the nonrelativistic case.

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[5] I. Waller, Zeits. f. Physik **38**, 635 (1926) solves a similar problem involving associated Laguerre polynomials.

[6] E. T. Copson, reference 1, p. 259.

[7] W. N. Bailey, *Generalized Hypergeometric Series* (Cambridge Tract No. 32, 1935), p. 18.

[8] S. Pasternack, Proc. Nat. Acad. Sci. **23**, 91 (1937).