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Relativistic hydrogen atom in the momentum representation

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The Dirac equation for the hydrogen atom is solved exactly in momentum space chosen to be properly conjugate to the spherical polar variables of position space. The coupled first-order differential equations are readily solved to give functions which involve a sum over poles along the imaginary axis at iZp_0/N, where N is the apparent principal quantum number.

INTRODUCTION

In recent work we have shown[1] that the wave functions for the hydrogen atom originally obtained by Podolsky and Pauling[2] were not in fact truly expressed in momentum space. Their functions were obtained by direct Fourier transformation from position space to a space in which the variables are P,Θ,Φ, representing the total momentum and its polar-angular coordinates as measured from the same axes as r,θ,ϕ, the position-space electronic coordinates. However, these momenta are not conjugate to any of the relevant spatial variables. This difficulty was only recently pointed out[1] so that in the meantime a considerable body of calculations in many systems including both atoms and molecules was carried out in this improper representation.[3] Rubinowitz[4] utilized the same transformation as Podolsky and Pauling to obtain wave functions related to the solutions of the Dirac equations. Levy[5] obtained the same results by solving directly the Dirac equation expressed in the above representation. Van Hove[6] used this same representation in solving for relativistic corrections for nucleon interactions utilizing the momentum analog of the meson potential.

In this work we shall obtain the Dirac equations in the momentum representation using variables p,p_θ,p_ϕ which have been chosen properly conjugate to the appropriate position-space variables. We shall show that an exact solution may be obtained with surprisingly little effort, analogous to the nonrelativistic momentum-space equations. Not only that, but the eigenfunctions of the radial momentum p are shown to be rather simple finite sums over poles of various orders in the complex plane. This property has been found to be of considerable value in nonrelativistic calculations in helium[7,8] since integration over wave functions is made quite simple by using the theory of residues. It is expected that similar simplifications will result from calculations with the relativistic functions derived here.

MOMENTUM SPACE IN SPHERICAL SYMMETRY

It is generally assumed that wave functions in position space may be transformed into momentum space using a simple Fourier transform. However, this is generally true only for Cartesian coordinates. It can be shown that for spherical polar coordinates, the transform which preserves the conjugate character of the variables is not a Fourier transform.[1] Furthermore, in order to maintain consistent quantum-mechanical uncertainty relations it is useful to utilize the variables r,v,t which are related to r,θ,ϕ by the relations

$$v=e^{i\phi},\quad t=e^{i\pi\cos\theta}.$$

If we then choose our momentum operators p,p_θ,p_ϕ such that

$$p=-i\left[\frac{\partial}{\partial r}+\frac{1}{r}\right],\quad p_\theta=\pi t\frac{\partial}{\partial t},$$

$$p_\phi=v\frac{\partial}{\partial v},$$

we then have the commutation and uncertainty relations

$$[p,r]=i,\quad \Delta p\,\Delta r\geq\tfrac{1}{2};$$

$$[p_\theta,t]=\pi t,\quad \Delta p_\theta \Delta t \geq \tfrac{1}{2}\pi[1-(\Delta t)^2]^{1/2};$$

$$[p_\phi,v]=v,\quad \Delta p_\phi \Delta v \geq \tfrac{1}{2}[1-(\Delta v)^2]^{1/2}.$$

With this choice we may then relate momentum-space functions to position-space functions by the transformation

$$\phi(p,p_\theta,p_\phi)$$
$$=(2\pi)^{-3/2}\int_0^\infty\int_{-1}^{1}\int_1^{e^{\pi i}} S(\vec{p},\vec{q})\psi(r,t,v)d\tau,$$

where

$$d\tau=\pi^{-1}r^2dr\,d\ln t\,d\ln v$$

and

$$S(\vec{p},\vec{q})=\left[\frac{2}{\pi}\right]^{1/2}\frac{1}{r}\exp(irp+\pi^{-1}p_\theta\ln t+p_\phi\ln v).$$

Note the most important difference between this and a Fourier transform is the factor of r^{-1}. This has the advantage of preserving the reciprocal relationship between the operator r and r^{-1} in momentum space:

$$r=i\frac{d}{dp},\quad r^{-1}=-i\int dp\equiv \underline{I},$$

where the lower limit of integration is chosen so that integration constants vanish. This latter choice is necessary to ensure that r and r^{-1} commute.

DIRAC EQUATION FOR THE HYDROGEN ATOM

It is easy to show[9] that the four components of the Dirac wave function for hydrogen may be written

$$u_1=\hat{g}(r)\left[\frac{l+m+\frac{1}{2}}{2l+1}\right]^{1/2}Y_{l,m-1/2}(\theta,\phi),$$

$$u_2=-\hat{g}(r)\left[\frac{l-m+\frac{1}{2}}{2l+1}\right]^{1/2}Y_{l,m+1/2}(\theta,\phi),$$

$$u_3=-i\hat{f}(r)\left[\frac{l-m+3/2}{2l+3}\right]^{1/2}Y_{l+1,m-1/2}(\theta,\phi),$$

$$u_4=-i\hat{f}(r)\left[\frac{l+m+3/2}{2l+3}\right]^{1/2}Y_{l+1,m+1/2}(\theta,\phi).$$

Since the angular factors are identical to the non-relativistic results, we may readily show that in momentum space the solutions are the same as previously derived,[1] namely,

$$\rho_m(p_\phi)=\delta(p_\phi+m),$$

$$\beta_l^m(p_\theta)=\sum_{j=E(m/2)}^{E(l/2)} a_j p_\theta^{-(m+1)/2}J_{j-(m-1)/2}(p_\theta),$$

where $J_n(p_\theta)$ are Bessel functions. The only remaining functions to be determined are $\hat{f}(r)$ and $\hat{g}(r)$ for which the Dirac equations may be written[9]

$$\frac{d\hat{g}}{dr}+(1+x)\frac{\hat{g}}{r}=\left[E_0+E+\frac{Z\alpha}{r}\right]\hat{f},$$

$$\frac{d\hat{f}}{dr}+(1-x)\frac{\hat{f}}{r}=\left[E_0-E-\frac{Z\alpha}{r}\right]\hat{g},$$

where $x=-(l+1)$ for $j=l+\frac{1}{2}$ and $x=+l$ for $j=l-\frac{1}{2}$. We have used $\alpha=e^2/\hbar c$ as the fine-structure constant, and a factor of $(\hbar c)^{-1}$ has been absorbed in E and E_0 for convenience. Transforming to momentum space,

$$\hat{f}(r)\rightarrow f(p),$$

$$\hat{g}(r)\rightarrow g(p),$$

$$i\left[\frac{d}{dr}+\frac{1}{r}\right]\rightarrow p,$$

$$\frac{1}{r}\rightarrow -i\int dp\equiv \underline{I},$$

we obtain

$$pg+ix\underline{I}g=[i(E_0+E)+Z\alpha i\underline{I}]f,$$

$$pf-ix\underline{I}f=[i(E_0-E)-Z\alpha i\underline{I}]g.$$

At this point it is convenient to define the parameter γ which we will later show to equal $[x^2-(Z\alpha)^2]^{1/2}$. Note that γ is not necessarily an integer, but using the rules for fractional derivatives[10] we may take the $(\gamma-1)$th derivative, and defining $G=g^{(\gamma-2)}$, $F=f^{(\gamma-2)}$ we obtain

$$pG'+(\gamma-1+x)G=i(E_0+E)F'+Z\alpha F,$$

$$pF'+(\gamma-1-x)F=i(E_0-E)G'-Z\alpha G,$$

using the substitution

$$F=(1-\epsilon)^{1/2}(\chi_1+\chi_2),$$

$$G=(1+\epsilon)^{1/2}(\chi_1-\chi_2),$$

where $\epsilon=E/E_0$, and by taking first the sum then the difference of the resultant equations, we obtain

$$[p-iE_0(1-\epsilon^2)^{1/2}]\chi_1'+\left[\gamma-1+\frac{Z\alpha\epsilon}{(1-\epsilon^2)^{1/2}}\right]\chi_1=\left[x+\frac{Z\alpha}{(1-\epsilon^2)^{1/2}}\right]\chi_2,$$

$$[p-iE_0(1-\epsilon^2)^{1/2}]\chi_2'+\left[\gamma-1-\frac{Z\alpha\epsilon}{(1-\epsilon^2)^{1/2}}\right]\chi_2=\left[x+\frac{Z\alpha}{(1-\epsilon^2)^{1/2}}\right]\chi_1 ;$$

letting $\kappa=E_0(1-\epsilon^2)^{1/2}=E_0Z\alpha/N$, where N is to be determined, we write

$$(p-i\kappa)\chi_1'+(\gamma-1+N\epsilon)\chi_1=(x+N)\chi_2 ,$$

$$(p+i\kappa)\chi_2'+(\gamma-1-N\epsilon)\chi_2=(x-N)\chi_1 .$$

These coupled first-order differential equations have the solution

$$\chi_1=C\frac{(p+i\kappa)^m}{(p-i\kappa)^n} ,$$

$$\chi_2=\frac{1}{C}\frac{(p-i\kappa)}{(p+i\kappa)}\chi_1 ,$$

where C is a constant. Substituting, we obtain

$$\left[m-n+\gamma-1+N\epsilon-\frac{x+N}{C}\right]p+\left[-(m+n)+\gamma-1+N\epsilon+\frac{x+N}{C}\right]i\kappa=0 ,$$

$$[m-n+\gamma-1-N\epsilon-(x-N)C]p+[-(m+n+2)-(\gamma-1-N\epsilon)-(x-N)C]i\kappa=0 .$$

These two algebraic equations have the solution

$$m=\frac{x+N}{C} \quad \text{and} \quad N\epsilon=m+\gamma .$$

Substituting these results into the equations, we obtain

$$(p-i\kappa)\chi_1'+(2\gamma-1+m)\chi_1=(x+N)\chi_2 ,$$

$$(p+i\kappa)\chi_2'-(m+1)\chi_1=(x-N)\chi_1 ,$$

$$[(m-n)p-(m+n)i\kappa+(2\gamma-1+m)(p+i\kappa)]\chi_1=(x+N)(p+i\kappa)\chi_2 ,$$

$$[(m-n)p-(m+n+2)i\kappa-(m+1)(p-i\kappa)]\chi_2=(x-N)(p-i\kappa)\chi_1 .$$

Solving these equations with some simple algebra, we obtain

$$m=n-2\gamma+1 ,$$

$$N^2-x^2=(n+1)(n-2\gamma+1) ,$$

and, letting $n'=n-2\gamma+1$,

$$\epsilon=\frac{n'+\gamma}{N} .$$

At this point by using the relation between $(1-\epsilon^2)^{1/2}$ and $Z\alpha/N$, it is easy to show $\gamma^2=x^2-(Z\alpha)^2$. The solutions now are

$$\chi_1=\frac{x+N}{n'}\frac{(p+i\kappa)^{n'}}{(p-i\kappa)^{n'+2\gamma-1}} ,$$

$$\chi_2=\frac{(p+i\kappa)^{n'+1}}{(p-i\kappa)^{n'+2\gamma}} .$$

Remembering the definition of f and g above, we must integrate these $\gamma-2$ times,[10] obtaining finally

$$f=(1-\epsilon)^{1/2}\frac{(-1)^{3\gamma}}{(i\kappa)^{2\gamma+2}}\sum_{k=0}^{n'+1}\left[\frac{x+N}{n'}\frac{n'-k+1}{n'+1}+1\right]\times\frac{a_k(i\kappa)^k}{(p-i\kappa)^{\gamma+k+1}} ,$$

$$g=(1+\epsilon)^{1/2}\frac{(-1)^{3\gamma}}{(i\kappa)^{2\gamma+2}}\sum_{k=0}^{n'+1}\left[\frac{x+N}{n'}\frac{n'-k+1}{n'+1}-1\right]\times\frac{a_k(i\kappa)^k}{(p-i\kappa)^{\gamma+k+1}} ,$$

where

$$a_k=\frac{2^k\Gamma(n'+2)\Gamma(\gamma+k+1)}{\Gamma(k+1)\Gamma(n'-k+2)\Gamma(2\gamma+k+1)}$$

and the quantum condition $n'=$an integer arises from the requirement that $f,g\to 0$ as $p\to\infty$.

DISCUSSION

The expression for ϵ is, of course, the same as that obtained in position space. The wave functions, however, are considerably simpler than the sums of hypergeometric functions or Laguerre polynomials obtained in other representations.[4,5,9,11] The functions derived above have poles at

$$i\kappa = iE_0(1-\epsilon^2)^{1/2} = \frac{iZp_0}{N} ,$$

where $p_0 = me^2/\hbar^2$. Note this is exactly the same as for the nonrelativistic hydrogen atom[1] except n' is replaced by the "apparent principal quantum number"

$$N = (n'^2 + 2n'\gamma + x^2)^{1/2} .$$

For unbound states where $\epsilon \geq 1$ or $\epsilon \leq -1$, N is pure imaginary, and the singularity lies along the real axis, at a point corresponding to the excess momentum above the rest momentum. For $0 \leq \epsilon < 1$ we have bound states with κ real and singularity along the imaginary axis. For states with $\epsilon < 0$ we enter the region where $Z\alpha > |x|$, and our solutions break down mathematically since γ becomes imaginary. In position space this problem may be eliminated by corrections for the finite size of the nucleus.[12,13] In momentum space the analogous potential introduces the exponential integral function into the equations for $f(p), g(p)$, vastly complicating their solution. Since states with $\epsilon < 0$ have important consequences for vacuum polarization and positron creation in quantum electrodynamics, it would be of interest to pursue this further and will be the basis for future investigation.

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