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# The relativistic hydrogen atom: A simple solution

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In his well-known textbook on quantum mechanics,[1] Schiff shows that the relativistic Schrödinger equation, also known as the Klein-Gordon (KG) equation, can be reduced, in the case of the Coulomb potential, to a form nearly identical to that of the nonrelativistic (NR) Schrödinger equation for the same potential. As a result the eigenfunctions and eigenvalues of the bound states can be inferred immediately from the known solutions of the NR problem. Here we show that an analogous procedure leads to the solutions of the Dirac equation for the hydrogen atom. The standard solution of the problem is considerably more complicated.[2,3]

We proceed as follows: After reminding the reader of Schiff's treatment of the relativistic bound-state Coulomb problem for a spin-zero particle, we show how the Dirac equation can be put into a form analogous to the KG equation. Separating in spherical coordinates (for a central potential), the angular eigenvalue problem is solved, the eigenfunctions being two component spinors. The radial eigenfunctions and energy for the hydrogen atom are immediately inferred from the solutions of the NR Schrödinger equation. Each eigenfunction of the energy and angular momentum depends upon only a *single* radial function. Our solutions are not parity eigenstates; nevertheless they can be used directly for calculating atomic properties. An Appendix discusses relevant properties of the associated Laguerre functions and of the angular eigenfunctions; it shows the relation of our solutions to the standard (parity eigenstate) solutions.

To show the simplicity of Schiff's argument (and to establish the notation), we review his treatment of the KG equation. With natural units ($\hbar = c = 1$), the KG equation for a negative charge in an electromagnetic field is

$$(\pi^\mu \pi_\mu - m^2)U(\mathbf{r}) = 0, \tag{1}$$

where $\pi_\mu = i\partial/\partial x^\mu + eA_\mu$. Specializing to the Coulomb case where $A_0 = +Ze/r$ and $\mathbf{A} = 0$, Eq. (1) simplifies (for stationary states) to

$$(-\nabla^2 + m^2)U(\mathbf{r}) = (E + \gamma/r)^2 U(\mathbf{r}), \tag{2}$$

where $\gamma \equiv Ze^2$. In spherical coordinates this becomes

$$\left[\frac{1}{\rho^2}\frac{\partial}{\partial\rho}\rho^2\frac{\partial}{\partial\rho} + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{L^2 - \gamma^2}{\rho^2}\right)\right] U(\mathbf{r}) = 0, \tag{3}$$

where $\lambda = 2E\gamma/\alpha$ and $\rho = \alpha r$, with $\alpha = 2(m^2 - E^2)^{1/2}$. Note that $E = m/(1 + \gamma^2/\lambda^2)^{1/2}$. $L^2$ is the square of the usual angular momentum operator whose eigenstates are $Y_{lm}(\theta,\varphi)$ with eigenvalues $l(l+1)$. Thus, introducing $U(\mathbf{r}) = R(r)Y_{lm}$, we have

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right) + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1) - \gamma^2}{\rho^2}\right) R = 0. \tag{4}$$

Except for the $-\gamma^2/\rho^2$ term, Eq. (4) is identical in form to the NR Schrödinger equation. (Of course, in that case $E = -m\gamma^2/2\lambda^2$ and is the binding energy.) Hence, if we define $s = \frac{1}{2}[(2l+1)^2 - 4\gamma^2]^{1/2} - \frac{1}{2}$, Eq. (4) can be written

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right) + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{s(s+1)}{\rho^2}\right) R = 0, \tag{5}$$

and is identical in form to the NR Schrödinger equation. By comparison with the latter, the solutions of Eq. (5) are

$$R(\rho) = \rho^s e^{-\rho/2} L^{2s+1}_{\lambda-s-1}(\rho). \tag{6}$$

The eigenvalue spectrum $\lambda = n - l + s$, where $n = l+1, l+2, \cdots$ (i.e., $\lambda = s+1, s+2, \cdots$), is obtained by requiring $R(\rho)$ to be well behaved at $\rho = 0$ and $\rho = \infty$. With these values, $(\lambda - s - 1)$ takes on integer values and the Laguerre functions $L^{2s+1}_{\lambda-s-1}$ are polynomials in $\rho$ of order $\lambda - s - 1$. A discussion of their properties can be found in the Appendix. Summarizing, we have found

$$E_{n,l} = m/[1 + \gamma^2/(n - l + s)^2]^{1/2}, \tag{7}$$

with

$$U_{nlm}(r) = (\alpha r)^s e^{-\alpha r/2} L^{2s+1}_{n-l-1}(\alpha r), \tag{8}$$

for $n = 1,2,3,\cdots$; $l = 0,1,\cdots(n-1)$. These results were all obtained by direct comparison with the NR Schrödinger case.

To perform an analogous reduction of the Dirac equation

$$(\gamma_\mu \pi^\mu - m)\psi = 0, \tag{9}$$

we introduce projection operators $P_1 = (\frac{1}{2})(1 + \gamma_5)$ and $P_2 = (\frac{1}{2})(1 - \gamma_5)$, with $\gamma_5^2 = 1$. The operators obey $P_1^2 = P_1$, $P_2^2 = P_2$, $P_1P_2 = P_2P_1 = 0$, and they satisfy $P_1\gamma^\mu = \gamma^\mu P_2$. Applying $P_2$ to Eq. (9) and defining

$$\psi_1 \equiv P_1\psi, \quad \psi_2 = P_2\psi, \tag{10}$$

we get

$$\psi_2 = m^{-1}P_2\gamma_\mu\pi^\mu\psi = m^{-1}\gamma_\mu\pi^\mu\psi_1. \tag{11}$$

Since $P_1 + P_2 = I$,

$$\psi = \psi_1 + \psi_2 = m^{-1}(\gamma_\mu\pi^\mu + m)\psi_1. \tag{12}$$

Given $\psi$, one can find $\psi_1$ using Eq. (10); given $\psi_1$, one can recover $\psi$ by using Eq. (12). Evidently, using Eqs. (9) and (12), $\psi_1$ satisfies the equation

$$(\gamma_\nu\pi^\nu - m)(\gamma_\mu\pi^\mu + m)\psi_1 = 0. \tag{13}$$

In the standard representation (using $2\times 2$ block matrix notation), we have

$$\gamma_5 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad P_1 = \frac{1}{2}\begin{pmatrix} I & I \\ I & I \end{pmatrix},$$

so that $\psi_1$ takes the form

$$\psi_1 = \begin{pmatrix} V \\ V \end{pmatrix}, \tag{14}$$

where $V$ is a two-component vector. Writing out Eq. (13) for stationary states, we find

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$$\frac{1}{\rho^2}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial}{\partial\rho}\right)V + \left(\frac{\lambda}{\rho}-\frac{1}{4}-\frac{L^2-\gamma^2-i\gamma\sigma\cdot\hat{\rho}}{\rho^2}\right)V=0, \quad (15)$$

where $\lambda$ and $\rho$ are defined just as after Eq. (3). We have used the standard representation in which

$$\gamma^0=\begin{pmatrix} I & 0\\ 0 & -I\end{pmatrix},\ \gamma=\begin{pmatrix} 0 & \sigma\\ -\sigma & 0\end{pmatrix}$$

and the $\{\sigma_i\}$ are the usual Pauli matrices.[4] Evidently, we have omitted the unit matrix in terms such as $\lambda/\rho$, etc. Equation (15) bears a striking resemblance to Eq. (3) except for the nondiagonal piece $i\gamma\sigma\cdot\hat{\rho}/\rho^2$.

Equation (15) is easily diagonalized in terms of the usual angular functions $\varphi^{\pm}_{jm}$, which are eigenstates of $J^2$, $J_z$, $L^2$, and $S^2$. ($\mathbf{J}\equiv\mathbf{L}+\sigma/2$). These two-component vectors have $s=\frac{1}{2}$ and $l=j\mp\frac{1}{2}$ (and the parity of $l$). We discuss the $\varphi^{\pm}_{jm}$ in the Appendix, but for the present discussion we shall need only the property

$$\sigma\cdot\hat{\rho}\varphi^{\pm}_{jm}=\varphi^{\mp}_{jm}. \quad (16)$$

This follows from the fact that $\sigma\cdot\hat{\rho}$ is a pseudoscalar operator; it commutes[5] with $\mathbf{J}$, and $(\sigma\cdot\hat{\rho})^2=I$. Hence, $\sigma\cdot\hat{\rho}$ changes parity but not $j$ and $m$.

We now introduce

$$G^{\pm}_{jm}\equiv\varphi^{\pm}_{jm}+x_{\pm}\varphi^{\mp}_{jm}, \quad (17)$$

with $x_{\pm}=(\pm i/\gamma)[(j+\frac{1}{2})-k)]$ where $k\equiv[(j+\frac{1}{2})^2-\gamma^2]^{1/2}$. It is easy to check that these functions satisfy

$$(L^2-\gamma^2-i\gamma\sigma\cdot\hat{\rho})\,G^{\pm}_{jm}=S_{\pm}(S_{\pm}+1)G^{\pm}_{jm} \quad (18)$$

with $S_{\pm}=(k-\frac{1}{2})\mp\frac{1}{2}$. Note that $x_{\pm}$ are of order $\gamma$ so that the $G^{\pm}_{jm}$ are *approximate* eigenstates of parity. Writing $V(\rho,\theta,\varphi)=V^{\pm}(\rho)G^{\pm}_{jm}(\theta,\varphi)$, where $V^{\pm}(\rho)$ are ordinary functions, Eq. (15) becomes

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dV^{\pm}}{d\rho}\right) + \left(\frac{\lambda}{\rho}-\frac{1}{4}-\frac{S_{\pm}(S_{\pm}+1)}{\rho^2}\right)V^{\pm}(\rho)=0. \quad (19)$$

By comparison with Eq. (5), we may now immediately write

$$V^{\pm}(\rho)=\rho^{S_{\pm}}e^{-\rho/2}L^{2S_{\pm}+1}_{\lambda-S_{\pm}-1}(\rho). \quad (20)$$

Again $\lambda$ must be $S_{\pm}+1, S_{\pm}+2,\cdots$ to satisfy the boundary conditions. If we introduce the usual principal quantum number, $n=\lambda+(j+\frac{1}{2})-k$, then

$$E_{n,j}=m/\{1+\gamma^2/[n+k-(j+\tfrac{1}{2})]^2\}^{1/2}, \quad (21)$$

$$V^{+}(\rho)=\rho^{k-1}e^{-\rho/2}L^{2k-1}_{n-(j+1/2)}, \quad (22)$$

$$V^{-}(\rho)=\rho^{k}e^{-\rho/2}L^{2k+1}_{n-(j+1/2)-1}, \quad (23)$$

for $n=1,2,3,\cdots$; $j=\frac{1}{2},3/2,\cdots,n-\frac{1}{2}$, except that $V_{-}(\rho)$ does not exist for the maximum $j$ value.

In conclusion, we have found that the hydrogen atom states of energy $E_{n,j}$ are, for $j<n-\frac{1}{2}$,

$$\psi^{\pm}_{n,jm}=V^{\pm}_{nj}(\rho_{nj})G^{\pm}_{jm}(\theta,\varphi), \quad (24)$$

with

$$\rho_{nj}=2m\gamma r[(n+k-1)^2+\gamma^2]^{-1/2}. \quad (25)$$

For $j=n-\frac{1}{2}$ there is only one state, namely $\psi^{+}_{njm}$, as given by Eq. (24).

## APPENDIX

In this Appendix we discuss a few details of our presentation which are useful for calculative purposes but not essential to the mainstream of the derivation.

### A. Definition and properties of the Laguerre equation (Ref. 6)

In the Schrödinger, Klein-Gordon, and Dirac cases the radial wave equation reduces to the form

$$\frac{1}{z^2}\frac{d}{dz}\left(z^2\frac{df}{dz}\right)+\left(\frac{\lambda}{z}-\frac{1}{4}+\frac{a(a+1)}{z^2}\right)f=0. \quad (A1)$$

With the substitution $f(z)=z^a e^{-z/2}F(z)$, we obtain

$$\frac{d^2F}{dz^2}+\left(\frac{2(a+1)}{z}-1\right)\frac{dF}{dz}+\left(\frac{\lambda-a-1}{z}\right)F=0. \quad (A2)$$

This is the well-known special case of the confluent hypergeometric equation that is called the Laguerre equation. It is usually written

$$\frac{d^2L^{\alpha}_n}{dz^2}+\left(\frac{\alpha+1}{z}-1\right)\frac{dL^{\alpha}_n}{dz}+\frac{n}{z}L^{\alpha}_n=0, \quad (A3)$$

where $L^{\alpha}_n(z)$ is the notation used for the regular solutions. These are polynomials for integer values of $n$ and for all values of $\alpha$. They are given by

$$L^{\alpha}_n(z)=\sum_{m=0}^{n}\frac{\Gamma(n+\alpha+1)}{\Gamma(n-m+1)\Gamma(\alpha+m+1)}\frac{(-z)^n}{\Gamma(m+1)}; \quad (A4)$$

for example, $L^{\alpha}_0=1$, $L^{\alpha}_1=\alpha+1-z$, etc.

### B. Definition and properties of the spinor spherical harmonics

We wish to construct eigenstates of $J^2$, $J_z$, $L^2$, and $S^2$. In our representation, $\mathbf{S}=\sigma/2$ and $\mathbf{L}$ is the usual differential operator in ordinary three-dimensional space. The eigenfunctions of $S^2$ and $S_z$ are the spinors

$$\chi_{1/2,1/2}=\begin{pmatrix}1\\0\end{pmatrix} \quad\text{and}\quad \chi_{1/2,-1/2}=\begin{pmatrix}0\\1\end{pmatrix},$$

where $S^2\chi_{1/2,q}=(3/4)\chi_{1/2,q}$ and $S_z\chi_{1/2,q}=q\chi_{1/2,q}$. The eigenfunction of $L^2$ and $L_z$ are the usual spherical harmonics, $Y_{l,p}(\theta,\varphi)$, where

$$L^2Y_{l,p}(\theta,\varphi)=l(l+1)Y_{l,p} \quad\text{and}\quad L_zY_{l,p}=pY_{l,p}.$$

To construct eigenstates of $J^2$ and $J_z$ we now couple these eigenfunctions via the usual Clebsch-Gordon coefficients and define

$$\varphi^{\pm}_{jm}\equiv\sum_{p,q}\langle l,p;\tfrac{1}{2},q\,|\,l,\tfrac{1}{2};jm\rangle Y_{l,p}(\theta,\varphi)\chi_{1/2,q}, \quad (B1)$$

where (+) and (−) refer to the two possibilities: $j=l\pm\frac{1}{2}$, respectively. Under the parity operation $\varphi^{\pm}_{jm}$ becomes $(-1)^{j\mp1/2}\varphi^{\pm}_{jm}$.

These functions are so simple that we write them out explicitly[7]

$$\varphi^{+}_{j,m} = \begin{bmatrix} [(j+m)/2j]^{1/2} Y_{j-1/2,m-1/2}(\theta,\varphi) \\ [(j-m)/2j]^{1/2} Y_{j-1/2,m+1/2}(\theta,\varphi) \end{bmatrix}, \quad \text{(B2)}$$

$$\varphi^{-}_{j,m} = \begin{bmatrix} [(j+1-m)/2(j+1)]^{1/2} Y_{j+1/2,m-1/2}(\theta,\varphi) \\ [(j+1+m)/2(j+1)]^{1/2} Y_{j+1/2,m+1/2}(\theta,\varphi) \end{bmatrix}. \quad \text{(B2b)}$$

The property used in the text, $\sigma\cdot\hat{\rho}\varphi^{\pm}_{j,m} = \varphi^{\mp}_{j,m}$, can be verified directly by using

$$\sigma\cdot\hat{\rho} = \left(\frac{3}{4\pi}\right)^{1/2} \begin{bmatrix} Y_{1,0} & \sqrt{2}\, Y_{1,-1} \\ \sqrt{2}\, Y_{1,+1} & -Y_{1,0} \end{bmatrix}. \quad \text{(B3)}$$

### C. Connection with usual solutions to the hydrogen atom

From our results for $\psi_1$, namely, that

$$\psi^{\pm}_1 = \begin{pmatrix} V^{\pm}G^{\pm} \\ V^{\pm}G^{\pm} \end{pmatrix},$$

we can recover the usual type Dirac spinor by using Eq. (12), i.e.,

$$\psi^{\pm} \equiv (1/m)(\gamma_\mu \pi^\mu + m)\psi^{\pm}_1. \quad \text{(C1)}$$

For a given $n$ value, the maximum $j$ value has only the (+) solution (i.e., there is no energy degeneracy) so that Eq. (C1) will produce a multiple of the usual solution. Since for other $j$ values we have two solutions for each energy eigenvalue, this inversion does not necessarily produce solutions which are parity eigenstates. In fact, because we have introduced the $G^{\pm}$ angular functions, Eq. (C1) will not directly produce parity eigenstates. However, it is easy to form the proper linear combinations of these two solutions in order to recover the conventional results.

For the usual spinors of Eq. (C1), parity eigenstates are those spinors whose upper and lower components are multiples of $\varphi^{\pm}$. If we write

$$\psi^{\pm}_p = \psi^{\pm} + B_{\pm}\psi^{\mp}, \quad \text{(C2)}$$

where $\psi^{\pm}_p$ are parity eigenstates then, by using the relation between the $G^{\pm}$ and $\varphi^{\pm}$, one can verify that

$$B_+ = i(m^2 - E^2)^{1/2}/[E(j+\tfrac{1}{2}) + mk] \quad \text{(C3)}$$

and

$$B_- = -i[E(j+\tfrac{1}{2}) - mk]/(m^2 - E^2)^{1/2}. \quad \text{(C4)}$$

(Note that $B_- = 0$ for $j = n - \tfrac{1}{2}$). Both $B_+$ and $B_-$ are of order $\gamma$ so that, for many purposes, $\psi^{\pm}$ may be used directly for calculations.


[1] Leonard I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1968), Chap. 13.

[2] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic, New York, 1957).

[3] A number of well-known quantum-mechanics texts derive the energy spectrum, but do not derive, or even quote, the eigenfunctions. For example, this is true of the books of Dirac, Schiff, Bethe and Jackiw, Bjorken and Drell, Trigg, Kursunoglu, Sakurai, Davydoff, Merzbacher, Kemble, and Messiah. A complete discussion is found, of course, in Ref. 2.

[4] An alternative derivation of Eq. (13) starts with the Dirac equation $(\pi_0 - \alpha\cdot\pi - \beta m)\psi = 0$. With $\alpha,\beta$ in the standard representation, write this equation as 2 two-component equations; add and subtract the latter to obtain $(\pi_0 \pm \sigma\cdot\pi)(\pi_0 \mp \sigma\cdot\pi)\chi_\pm \equiv m^2\chi_\pm$, where $\chi_\pm$ are two-component Paul spinors. For a full discussion of these equations see L. M. Brown, *Lectures in Theoretical Physics*, Vol. IV (Interscience, New York, 1962), p. 234.

[5] An elementary proof that $\mathbf{J} = \mathbf{L} + (\tfrac{1}{2})\sigma$ commutes with $\sigma\cdot\hat{\rho}$ goes as follows: Let $\hat{\rho} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ and $L_3 = -i\partial/\partial\varphi$. Then $[L_3,\hat{\rho}] = i(\sin\theta\ \sin\varphi, -\sin\theta\cos\varphi, 0)$ and $(\tfrac{1}{2})[\sigma_3,\sigma] = i(\sigma_y, -\sigma_x, 0)$; hence $[J_3,\sigma\cdot\hat{\rho}] = \sigma\cdot[L_3,\hat{\rho}] + (\tfrac{1}{2})[\sigma_3,\sigma]\cdot\hat{\rho} = 0$. The result for the other components of $\mathbf{J}$ follows from rotational invariance.

[6] For additional properties see, e.g., P. M. Morse and H. Feshbach, *Methods of Theoretical Physics, Part I* (McGraw-Hill, New York, 1953), p. 784.

[7] See, e.g., J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964), p. 53.


# Group problem-solving sessions in PSI physics courses


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## INTRODUCTION

Much discussion of the Keller procedure or Personalized System of Instruction (PSI) has been concerned with what some people contend is the impersonal mechanical nature of putting the student on his own with the textbook. People have argued that a PSI course robs the student of a chance for interaction with the instructor. Proponents counter by saying that the situation is quite the contrary. They contend that PSI allows instructors to get to know their students better as individuals.[1] Even if the proponents are correct in their contentions that PSI actually promotes better student-instructor interaction, there is still a lack of student-student interaction. This is a matter which the students themselves often criticize in such courses.

## GENERAL IDEA

The modification proposed here will be developed within the context of teaching introductory physics courses, although, as will be shown later, it is by no means limited to such courses. The modification is to institute problem sessions in which the instructor works example problems relating to a particular topic on a periodic basis. Since the student already has his unit outlines to guide his study, the instructor can choose problems to expand on text material, clarify ideas or apply concepts from the unit. He can also concentrate on the processes of physics rather than its factual content. The student is required to attend each problem session, and the units are presented at a definite, steady pace throughout the term with each unit examined



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