

CHAPTER IV

RELATIVISTIC TWO DIMENSIONAL HYDROGEN ATOM

In this chapter the Dirac relativistic quantum mechanical treatment of the two dimensional hydrogen atom will be investigated. We start by first deriving the Dirac equation for the relativistic two dimensional hydrogen atom, then trying to find its solutions, restrict ourselves to the solutions which are simultaneous eigenfunctions of the Hamiltonian and the commuting constants of the motion. The results are then compared with the results already obtained for the nonrelativistic two dimensional hydrogen atom (Chapter III), and also with those for the three dimensional hydrogen atom (Chapter II) .

4.1 DERIVATION OF THE DIRAC EQUATION FOR THE TWO DIMENSIONAL HYDROGEN ATOM .

The Dirac equation for a spin- $\frac{1}{2}$ particle of rest mass m and electrical charge q in the presence of an electromagnetic field described by the scalar potential $A_0(\vec{r}, t)$ and the vector potential $\vec{A}(\vec{r}, t)$ is

$$H_{\text{Dirac}} U(\vec{r}, t) = \left[c\vec{\alpha} \cdot \left(\vec{p} - \frac{q}{c}\vec{A} \right) + \beta mc^2 + qA_0 \right] U(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} U(\vec{r}, t), \quad (4.1)$$

where A_0 and \vec{A} are evaluated at the position of the particle. Here \vec{p} stands for $-i\hbar\nabla$. This equation can be separated with respect to \vec{r} and t provided that the scalar and vector potentials are independent of time. By writing

$$U(\vec{r}, t) = U(\vec{r}) \exp(-iEt/\hbar) \quad , \quad (4.2)$$

we obtain

$$H_{\text{Dirac}} U(\vec{r}) = \left[c\vec{\alpha} \cdot \left(\vec{p} - \frac{q}{c} \vec{A} \right) + \beta mc^2 + qA_0 \right] U(\vec{r}) = EU(\vec{r}) , \quad (4.3)$$

which is referred to as the time-independent Dirac equation for a spin- $\frac{1}{2}$ particle in an electromagnetic field described by the time-independent scalar and vector potentials, $A_0(\vec{r})$ and $\vec{A}(\vec{r})$. The quantity E in the above equation is called the energy eigenvalue.

For the case of the two dimensional hydrogen atom, which is defined to be a system in which an electron moves around the nucleus in the xy -plane under the influence of an attractive Coulomb potential, by substituting into Eq.(4.3) the expressions

$$\begin{aligned} \vec{p} &= \hat{x}p_x + \hat{y}p_y , \\ q &= -e \end{aligned} \quad (4.4)$$

$$A_0 = \frac{Ze}{\rho} ; Z = \text{atomic number} ; \rho = \sqrt{(x^2 + y^2)} ,$$

and $\vec{A} = 0 ,$

we obtain the time-independent Dirac equation for the two dimensional atom

$$H_{\text{Dirac}} U(\vec{\rho}) = \left[c\alpha_x p_x + c\alpha_y p_y + \beta mc^2 - \frac{Ze^2}{\rho} \right] U(\vec{\rho}) = EU(\vec{\rho}) . \quad (4.5)$$

Thus we are dealing with the three matrices α_x , α_y , and β satisfying the relations

$$\begin{aligned} \alpha_i \alpha_j + \alpha_j \alpha_i &= 2\delta_{ij} \quad (i, j = x, y), \\ \alpha_i \beta + \beta \alpha_i &= 0 , \\ \beta^2 &= 1 . \end{aligned} \quad (4.6)$$

where δ_{ij} is the Kronecker symbol, which is defined as being 1 for $j=i$

and 0 for $i \neq j$;

$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}$$

The smallest dimension of the three matrices which satisfy Eqs.(4.6) is $N = 2$, i.e., the Pauli matrices δ_x^P , δ_y^P , and δ_z^P .

However, since we know that (a) in the nonrelativistic situation (Chapter III) the wave function of the electron, which is a particle of spin- $\frac{1}{2}$, has two components corresponding to the two possible orientations of the spin, and that (b) the effect of the relativistic generalization is to double the number of components of the wave function, we will choose α_x , α_y , and β to be 4-by-4 matrices.

In the usual representation, the Pauli representation, these matrices are

$$\alpha_x = \begin{bmatrix} 0 & \delta_x^P \\ \delta_x^P & 0 \end{bmatrix}, \quad \alpha_y = \begin{bmatrix} 0 & \delta_y^P \\ \delta_y^P & 0 \end{bmatrix}, \quad \text{and} \quad \beta = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}, \quad (4.7)$$

where δ_x^P and δ_y^P are Pauli's spin matrices

$$\delta_x^P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \delta_y^P = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad (4.8)$$

and I is the 2-by-2 unit matrix. An explicit form of Eq. (4.5) is, in this representation,

$$\begin{bmatrix} E - mc^2 + \frac{Ze^2}{\rho} & 0 & 0 & -c(p_x - ip_y) \\ 0 & E - mc^2 + \frac{Ze^2}{\rho} & -c(p_x + ip_y) & 0 \\ 0 & -c(p_x - ip_y) & E + mc^2 + \frac{Ze^2}{\rho} & 0 \\ -c(p_x + ip_y) & 0 & 0 & E + mc^2 + \frac{Ze^2}{\rho} \end{bmatrix} \begin{bmatrix} U^1(o) \\ U^2(o) \\ U^3(o) \\ U^4(o) \end{bmatrix} = 0. \quad (4.9)$$

4.2 SPIN AND CONSTANTS OF THE MOTION.

From the form of the Schroedinger wave equation,

$$HU(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} U(\vec{r}, t) \quad , \quad (4.10)$$

it follows that for any operator \mathcal{E} not involving the time explicitly (41) ;

$$\frac{d}{dt} \mathcal{E} = \frac{i}{\hbar} (H\mathcal{E} - \mathcal{E}H) = \frac{i}{\hbar} [H, \mathcal{E}] \quad . \quad (4.11)$$

Thus, by Eq.(4.11), constants of the motion exist for a set of commuting operators if and only if they commute with H. In connection with the angular momentum of the electron we first calculate the commutator of the orbital angular momentum L with the Hamiltonian H. Since , in our problem , the electron is confined to move only in the xy-plane, its orbital angular momentum L must be parallel to the z-axis, i.e.,

$$\vec{L} = \vec{r} \times \vec{p} = \hat{z} L_z \quad , \quad (4.12)$$

$$L_z = xp_y - yp_x = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \quad .$$

For the two dimensional relativistic hydrogen atom, in which the Hamiltonian is

$$H_{\text{Dirac}} = c\alpha_x p_x + c\alpha_y p_y + \beta mc^2 - \frac{Ze^2}{\rho} \quad , \quad (4.13)$$

the commutator of the orbital angular momentum with the Hamiltonian is

$$\begin{aligned} [L, H_{\text{Dirac}}] &= \hat{z} [L_z, H_{\text{Dirac}}] = \hat{z} c (\alpha_x [L_z, p_x] + \alpha_y [L_z, p_y]) \\ &= \hat{z} i\hbar c (\alpha_x p_y - \alpha_y p_x) \neq 0, \end{aligned} \quad (4.14)$$

where we have taken into account the facts that ;

- (a) L_z commutes with any symmetric function, this can be seen by noting that in the plane polar coordinates (ρ, ϕ) L_z takes the form $-i\hbar \frac{\partial}{\partial \phi}$,
- (b) βmc^2 , α_x , and α_y are constant matrices and so commute with L_z ,
- and (c) the commutator of the i^{th} component of the orbital angular momentum with the j^{th} component of the linear momentum satisfies the relation (42)

$$[L_i, p_j] = i\hbar p_k \quad , \quad (4.15)$$

i, j, k - cyclic permutation of x, y, z .

It follows then that the orbital angular momentum is not a constant of the motion.

However, we expect on the physical ground, i.e., rotational invariance of the system about the z -axis, that the z -component of the total angular momentum \vec{J} is a constant of the motion. This means that there must exist another operator, the so-called spin angular momentum \vec{S} , such that the sum of that operator with the orbital angular momentum can be interpreted as the total angular momentum and that its z -component is a constant of the motion.

The requirement that the z -component of the total angular momentum

$$J_z = L_z + S_z \quad (4.16)$$

is a constant of the motion implies the following conditions for S_z ;

$$[S_z, \alpha_x] = i\hbar \alpha_y \quad , \quad [S_z, \alpha_y] = i\hbar \alpha_x \quad , \quad [S_z, \beta] = 0 \quad . \quad (4.17)$$

Applying these conditions, we get

$$S_z = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & b+\hbar & 0 \\ 0 & 0 & 0 & a-\hbar \end{bmatrix}, \quad (4.18)$$

where a and b are any constants.

The values of a and b can be determined by recalling that in the case of nonrelativistic quantum mechanics the eigenvalues of the component of the angular momentum are

$$k, k-\hbar, k-2\hbar, \dots, -k+2\hbar, -k+\hbar, -k, \quad (4.19)$$

where k is the magnitude of the angular momentum (43). If we assume that the foregoing statement is also valid in the relativistic case then it follows that the values of the constants a and b must be $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$, respectively. Thus

$$S_z = \frac{1}{2}\hbar \begin{bmatrix} \sigma_z^P & 0 \\ 0 & \sigma_z^P \end{bmatrix} = \frac{1}{2}\hbar \sigma_z^D \quad (4.20)$$

where σ_z^P is the Pauli matrix

$$\sigma_z^P = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (4.21)$$

This implies that Eq.(4.9) is an equation which describe the two dimensional relativistic motion of a spin- $\frac{1}{2}$ particle of rest mass m , electric charge $q = -e$ under the influence of an attractive Coulomb potential.

Apart from the z-component of the total angular momentum J_z , there exists another operator which is also a constant of the motion and also commutes with J_z .

Let us consider first the spin-orbit coupling operator

$$\vec{S} \cdot \vec{L} = S_z L_z = \frac{1}{2} \hbar \sigma_z^D L_z, \quad (4.22)$$

the commutator of this operator with the Hamiltonian is

$$\begin{aligned} [\vec{S} \cdot \vec{L}, H_{\text{Dirac}}] &= \frac{1}{2} \hbar c \left\{ [\sigma_z^D L_z, \alpha_x p_x] + [\sigma_z^D L_z, \alpha_y p_y] \right\} \\ &\quad + \frac{1}{2} \hbar m c^2 [\sigma_z^D L_z, \beta] - \frac{1}{2} \hbar Z e^2 [\sigma_z^D L_z, \rho^{-1}] \\ &= \frac{1}{2} \hbar c \left\{ i \alpha_y (L_z p_x + p_x L_z) - i \alpha_x (L_z p_y + p_y L_z) \right\} \\ &\neq 0, \end{aligned} \quad (4.23)$$

where the relations

$$\begin{aligned} \sigma_z^D \alpha_x &= -\alpha_x \sigma_z^D = i \alpha_y, \\ \sigma_z^D \alpha_y &= -\alpha_y \sigma_z^D = -i \alpha_x, \\ \sigma_z^D \beta &= \beta \sigma_z^D, \end{aligned} \quad (4.24)$$

have been used. Thus, it is not a constant of the motion. However, as in the case of the three dimensional hydrogen atom (44), there is an operator related to $\sigma_z^D L_z$ which does commute with H_{Dirac} and with J_z . This is the operator

$$K = -\frac{\beta}{\hbar} \left(\sigma_z^D L_z + \frac{1}{2} \hbar \right). \quad (4.25)$$

Obviously K commutes with β and with any symmetric function.

Therefore, for the commutator with H_{Dirac} , consider

$$\begin{aligned}
[K, \alpha_x p_x + c \alpha_y p_y] &= -\frac{c}{\hbar} \left\{ [\beta \sigma_z^D L_z, \alpha_x p_x] + [\beta \sigma_z^D L_z, \alpha_y p_y] \right\} \\
&\quad - \frac{1}{2} c \left\{ [\beta, \alpha_x p_x] + [\beta, \alpha_y p_y] \right\} \\
&= -\frac{c}{\hbar} \left\{ [\beta \sigma_z^D L_z, \alpha_x p_x] + [\beta \sigma_z^D L_z, \alpha_y p_y] \right\} \\
&\quad - c (\beta \alpha_x p_x + \beta \alpha_y p_y) . \tag{4.26}
\end{aligned}$$

Since, with the help of Eqs. (4.6), (4.24) and (4.15),

$$\begin{aligned}
[\beta \sigma_z^D L_z, \alpha_x p_x] &= \beta \sigma_z^D \alpha_x L_z p_x - \alpha_x \beta \sigma_z^D p_x L_z \\
&= \beta (\sigma_z^D \alpha_x L_z p_x + \alpha_x \sigma_z^D p_x L_z) = i \beta \alpha_y [L_z, p_x] \\
&= -\beta \hbar \alpha_y p_y , \tag{4.27}
\end{aligned}$$

and, similarly,

$$[\beta \sigma_z^D L_z, \alpha_y p_y] = -\beta \hbar \alpha_x p_x , \tag{4.28}$$

we get

$$[K, c \alpha_x p_x + c \alpha_y p_y] = 0 , \tag{4.29}$$

that is, K commutes with H_{Dirac} . Since, by Eq.(4.24), β commutes with σ_z^D , it can be easily seen that the operator K commutes with J_z :

$$\begin{aligned}
[K, J_z] &= - \left[\frac{\beta}{\hbar} \sigma_z^D L_z + \frac{1}{2} \beta , L_z + \frac{1}{2} \hbar \sigma_z^D \right] \\
&= - \left(\frac{1}{\hbar} [\beta \sigma_z^D L_z, L_z] + \frac{1}{2} [\beta \sigma_z^D L_z, \sigma_z^D] + \frac{1}{2} [\beta, L_z] + \frac{\hbar}{4} [\beta, \sigma_z^D] \right) \\
&= 0 . \tag{4.30}
\end{aligned}$$

In the case of the relativistic two dimensional hydrogen atom we thus have the commuting constants of the motion

$$J_z = L_z + \frac{1}{2}\hbar\sigma_z^D \quad \text{and} \quad K = -\frac{\beta}{\hbar} \left(\sigma_z^D L_z + \frac{1}{2}\hbar \right), \quad (4.31)$$

so that in solving the eigenvalue equation (4.9) we may restrict ourselves to those eigenfunctions of H_{Dirac} that are simultaneously eigenfunctions of J_z and K .

4.3 THE SIMULTANEOUS EIGENFUNCTIONS OF THE CONSTANTS OF MOTION.

Written out more explicitly, the operator J_z is, in the plane polar coordinates (ρ, ϕ) ,

$$J_z = \hbar \begin{bmatrix} -i \frac{\partial}{\partial \phi} + \frac{1}{2} & 0 & 0 & 0 \\ 0 & -i \frac{\partial}{\partial \phi} - \frac{1}{2} & 0 & 0 \\ 0 & 0 & -i \frac{\partial}{\partial \phi} + \frac{1}{2} & 0 \\ 0 & 0 & 0 & -i \frac{\partial}{\partial \phi} - \frac{1}{2} \end{bmatrix} \quad (4.32)$$

If we denote the eigenvalues of J_z by $j\hbar$, then the corresponding eigenfunctions are

$$U_j(\rho, \phi) = \begin{bmatrix} U_j^1(\rho, \phi) \\ U_j^2(\rho, \phi) \\ U_j^3(\rho, \phi) \\ U_j^4(\rho, \phi) \end{bmatrix} = \frac{1}{\sqrt{2\pi}} \begin{bmatrix} R^1(\rho) \exp(i(j-\frac{1}{2})\phi) \\ R^2(\rho) \exp(i(j+\frac{1}{2})\phi) \\ R^3(\rho) \exp(i(j-\frac{1}{2})\phi) \\ R^4(\rho) \exp(i(j+\frac{1}{2})\phi) \end{bmatrix}, \quad (4.33)$$

where the constant factor $\frac{1}{\sqrt{2\pi}}$ is introduced for the further convenience. The possible values of j are determined from the condition of single-valueness, which requires that the wave functions $U_j(\rho, \phi)$ satisfy the equation

$$U_j(\rho, \phi+2\pi) = U_j(\rho, \phi) \quad (4.34)$$

This condition implies that

$$\exp(i(2\pi j)) = -1 ,$$

that is, we must restrict j to the values

$$j = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \pm\frac{7}{2}, \dots \quad (4.35)$$

In the plane polar coordinates (ρ, ϕ) , an explicit form of the operator K in the representation (4.7) is

$$K = \begin{bmatrix} i \frac{\partial}{\partial \phi} - \frac{1}{2} & 0 & 0 & 0 \\ 0 & -i \frac{\partial}{\partial \phi} - \frac{1}{2} & 0 & 0 \\ 0 & 0 & -i \frac{\partial}{\partial \phi} + \frac{1}{2} & 0 \\ 0 & 0 & 0 & i \frac{\partial}{\partial \phi} + \frac{1}{2} \end{bmatrix}, \quad (4.36)$$

By writing

$$U_j^A(\rho, \phi) = \begin{bmatrix} U_j^1(\rho, \phi) \\ 0 \\ 0 \\ U_j^4(\rho, \phi) \end{bmatrix} \quad \text{and} \quad U_j^B(\rho, \phi) = \begin{bmatrix} 0 \\ U_j^2(\rho, \phi) \\ U_j^3(\rho, \phi) \\ 0 \end{bmatrix}, \quad (4.37)$$

and operating on each of these U 's the operator K , we find that

$$\begin{aligned} KU_j^A(\rho, \phi) &= -jU_j^A(\rho, \phi), \\ KU_j^B(\rho, \phi) &= jU_j^B(\rho, \phi), \end{aligned} \quad (4.38)$$

i.e., $U_j^A(\rho, \phi)$ and $U_j^B(\rho, \phi)$ are the eigenfunctions of K belonging to the eigenvalues $k=-j$ and $k=j$, respectively. Thus, the eigenvalues of K are

$$k = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \pm\frac{7}{2}, \dots \quad (4.39)$$

This result can also be obtained by squaring Eq.(4.36) ;

$$K^2 = \left(-\frac{\beta}{\hbar} (6 \frac{D}{z} L_z + \frac{1}{2}\hbar)\right)^2 = \frac{1}{\hbar^2} J_z^2 .$$

Since the eigenvalues of J_z are $j\hbar$, the eigenvalues of K^2 are thus $k^2=j^2$ or $k=\pm j$.

Hence, there are two sets of functions which are the simultaneous eigenfunctions of J_z and K , one with $k=-j$ and the other with $k=j$;

$$U_{jk}^A(\rho, \phi) = \begin{bmatrix} R^1(\rho) \phi_j^1(\phi) \\ 0 \\ 0 \\ -iR^4(\rho) \phi_j^2(\phi) \end{bmatrix} , \quad (4.40)$$

and

$$U_{jk}^B(\rho, \phi) = \begin{bmatrix} 0 \\ R^2(\rho) \phi_j^2(\phi) \\ -iR^3(\rho) \phi_j^1(\phi) \\ 0 \end{bmatrix} , \quad (4.41)$$

where $\phi_j^1(\phi) = \frac{1}{\sqrt{2\pi}} \exp(i(j-\frac{1}{2})\phi) , \quad (4.42)$

$$\phi_j^2(\phi) = \frac{1}{\sqrt{2\pi}} \exp(i(j+\frac{1}{2})\phi) , \quad (4.43)$$

$$R^3(\rho) = -iR^3(\rho) , \quad (4.44)$$

and $R^4(\rho) = -iR^4(\rho) . \quad (4.45)$

The factor $(-i)$ is introduced to make the radial equations explicitly real.

4.4 THE RADIAL EQUATIONS .

Having computed the simultaneous eigenfunctions of J_z and K , we now proceed to consider the simultaneous eigenfunctions of J_z , K , and H_{Dirac} . In terms of the plane polar coordinates (ρ, ϕ) , the Dirac equation for the two dimensional hydrogen atom (4.9) takes the form

$$\begin{bmatrix} E - mc^2 + \frac{Ze^2}{\rho} & 0 & 0 & \hbar c e^{-i\phi} \left(i \frac{\partial}{\partial \rho} + \frac{1}{\rho} \frac{\partial}{\partial \phi} \right) \\ 0 & E - mc^2 + \frac{Ze^2}{\rho} & \hbar c e^{i\phi} \left(i \frac{\partial}{\partial \rho} - \frac{1}{\rho} \frac{\partial}{\partial \phi} \right) & 0 \\ 0 & \hbar c e^{-i\phi} \left(i \frac{\partial}{\partial \rho} + \frac{1}{\rho} \frac{\partial}{\partial \phi} \right) & E + mc^2 + \frac{Ze^2}{\rho} & 0 \\ \hbar c e^{i\phi} \left(i \frac{\partial}{\partial \rho} - \frac{1}{\rho} \frac{\partial}{\partial \phi} \right) & 0 & 0 & E + mc^2 + \frac{Ze^2}{\rho} \end{bmatrix} \begin{bmatrix} U^1(\vec{\rho}) \\ U^2(\vec{\rho}) \\ U^3(\vec{\rho}) \\ U^4(\vec{\rho}) \end{bmatrix} = 0, \quad (4.46)$$

this is because

$$\begin{aligned} p_x + ip_y &= -\hbar e^{i\phi} \left(\frac{\partial}{\partial \rho} - \frac{1}{\rho} \frac{\partial}{\partial \phi} \right), \\ \text{and} \\ p_x - ip_y &= -\hbar e^{-i\phi} \left(\frac{\partial}{\partial \rho} + \frac{1}{\rho} \frac{\partial}{\partial \phi} \right). \end{aligned} \quad (4.47)$$

For $U_{jk}^A(\rho, \phi)$, the above equation (4.46) splits up into the two radial equations

$$\begin{aligned} (E - mc^2 + \frac{Ze^2}{\rho}) R^1(\rho) + \hbar c \left\{ \frac{d}{d\rho} + \frac{1}{\rho} (j + \frac{1}{2}) \right\} R^4(\rho) &= 0, \\ (E + mc^2 + \frac{Ze^2}{\rho}) R^4(\rho) - \hbar c \left\{ \frac{d}{d\rho} - \frac{1}{\rho} (j - \frac{1}{2}) \right\} R^1(\rho) &= 0, \end{aligned} \quad (4.48)$$

or, since in this case $k = -j$,

$$\begin{aligned} (E - mc^2 + \frac{Ze^2}{\rho}) R^1(\rho) + \hbar c \left(\frac{d}{d\rho} - \frac{k}{\rho} + \frac{1}{2\rho} \right) R^4(\rho) &= 0, \\ (E + mc^2 + \frac{Ze^2}{\rho}) R^4(\rho) - \hbar c \left(\frac{d}{d\rho} + \frac{k}{\rho} + \frac{1}{2\rho} \right) R^1(\rho) &= 0. \end{aligned} \quad (4.49)$$



Similarly, for $U_{jk}^B(\rho, \phi)$, we obtain the radial equations

$$(E - mc^2 + \frac{Ze^2}{\rho})R^2(\rho) + \hbar c(\frac{d}{d\rho} - \frac{k}{\rho} + \frac{1}{2\rho})R^3(\rho) = 0, \quad (4.50)$$

$$(E + mc^2 + \frac{Ze^2}{\rho})R^3(\rho) - \hbar c(\frac{d}{d\rho} + \frac{k}{\rho} + \frac{1}{2\rho})R^2(\rho) = 0,$$

which are identical with Eqs.(4.49). Obviously, we can write

$$R^1(\rho) = R^2(\rho), \quad R^3(\rho) = R^4(\rho), \quad (4.51)$$

and it suffices to consider Eqs.(4.49).

4.5 SOLUTION OF RADIAL EQUATIONS FOR BOUND STATES ($0 < E < mc^2$).

By substituting for $R^1(\rho)$ and $R^4(\rho)$ in Eqs.(4.49) the expressions

$$R^1(\rho) = \rho^{-1/2} F(\rho) \quad \text{and} \quad R^4(\rho) = \rho^{-1/2} G(\rho), \quad (4.52)$$

we obtain* the well-known pair of couple first-order differential equations

$$\left(\frac{E - mc^2}{\hbar c}\right) + \frac{Z\alpha}{\rho} F(\rho) + \left(\frac{d}{d\rho} - \frac{k}{\rho}\right) G(\rho) = 0, \quad (4.53)$$

$$\left(\frac{E + mc^2}{\hbar c}\right) + \frac{Z\alpha}{\rho} G(\rho) - \left(\frac{d}{d\rho} + \frac{k}{\rho}\right) F(\rho) = 0,$$

where

$$\alpha = \frac{e^2}{\hbar c} \quad (4.54)$$

is the Sommerfeld fine structure constant.

To solve these two equations, we first examine the nature of the equations for the limits of small and large ρ , i.e., their

*since $\left(\frac{d}{d\rho} + \frac{1}{2\rho} \frac{k}{\rho}\right)\rho^{-1/2} P(\rho) = \rho^{-1/2}\left(\frac{d}{d\rho} \pm \frac{k}{\rho}\right)P(\rho)$, where $P(\rho)$ is any differentiable function of ρ .

asymptotic behaviors, and derive the conditions that the radial functions must satisfy in order that the probability density does not diverge anywhere within the range $\rho = 0$ and $\rho = \infty$. Then, the radial functions for all ρ are obtained by expanding the acceptable forms for them in power series.

4.5.1 Asymptotic Behaviors : For small ρ , $(\frac{E \pm mc^2}{\hbar c}) \ll \frac{Z\alpha}{\rho}$, the coupled radial equations (4.53) reduce to

$$\begin{aligned} \left(\frac{d}{d\rho} - \frac{k}{\rho} \right) G(\rho) + \frac{Z\alpha}{\rho} F(\rho) &= 0, \\ \left(\frac{d}{d\rho} + \frac{k}{\rho} \right) F(\rho) - \frac{Z\alpha}{\rho} G(\rho) &= 0. \end{aligned} \quad (4.55)$$

From these equations, we can solve for the separate second-order differential equations for $F(\rho)$ and $G(\rho)$; the resulting equations are

$$\left(\rho \frac{d^2}{d\rho^2} + \frac{d}{d\rho} - \frac{k^2}{\rho} + \frac{(Z\alpha)^2}{\rho} \right) \begin{Bmatrix} F(\rho) \\ G(\rho) \end{Bmatrix} = 0. \quad (4.56)$$

Assuming

$$\begin{Bmatrix} F(\rho) \\ G(\rho) \end{Bmatrix} \underset{\rho \rightarrow 0}{\sim} \rho^\gamma, \quad (4.57)$$

we get the condition

$$\gamma^2 = k^2 - (Z\alpha)^2. \quad (4.58)$$

However, the negative root of γ must be excluded, since it would make the functions $F(\rho)$ and $G(\rho)$ singular at the origin, and therefore make the probability densities diverge at $\rho = 0$. We thus get

$$\gamma_k = \sqrt{k^2 - (Z\alpha)^2}, \quad (4.59)$$

where the subscript k is added to denote the dependence of γ on k .

Substituting Eqs.(4.57) into Eqs.(4.52) yields

$$R(\rho) \underset{\rho \rightarrow 0}{=} \rho^{\gamma_k - \frac{1}{2}}, \quad (4.60)$$

that is, the radial wave functions behave like $\rho^{\gamma_k - \frac{1}{2}}$ near the origin. Since $R(\rho)$ is supposed to be finite at $\rho = 0$ (for the probability densities to be finite at the origin), we expect that γ_k is greater than or equal to $\frac{1}{2}$;

$$\gamma_k \geq \frac{1}{2}. \quad (4.61)$$

However, we shall admit values of γ_k slightly less than $\frac{1}{2}$, which correspond to $|k| = \frac{1}{2}$, since $(Z\alpha)$ is quite small that the value of $(\gamma_k - \frac{1}{2})$ is close to zero for interesting values of Z .

For large values of ρ , we can drop the $\frac{Z\alpha}{\rho}$ and the $\frac{k}{\rho}$ terms in Eqs.(4.53), which then reduced to the asymptotic forms

$$\begin{aligned} \frac{d}{d\rho} F(\rho) - \left(\frac{E + mc^2}{\hbar c}\right)G(\rho) &= 0, \\ \frac{d}{d\rho} G(\rho) + \left(\frac{E - mc^2}{\hbar c}\right)F(\rho) &= 0. \end{aligned} \quad (4.62)$$

Two features of the asymptotic forms of the radial functions may be noted from these equations. First, the two couple equations may be combined to obtain separate second-order equations for $F(\rho)$ and $G(\rho)$;

$$\left(\frac{d^2}{d\rho^2} - \lambda^2\right) \begin{Bmatrix} F(\rho) \\ G(\rho) \end{Bmatrix} = 0, \quad (4.63)$$

where λ is defined by

$$\lambda = \frac{((mc^2)^2 - E^2)^{\frac{1}{2}}}{\hbar c} = \frac{mc^2}{\hbar c} (1 - \epsilon^2)^{\frac{1}{2}} \quad (4.64)$$

with

$$\epsilon = \frac{E}{mc^2}. \quad (4.65)$$

Thus, the asymptotic forms (for large ρ) of the radial functions can be written as *

$$\begin{Bmatrix} F(\rho) \\ G(\rho) \end{Bmatrix} \rho \xrightarrow{\infty} \begin{Bmatrix} A \\ B \end{Bmatrix} e^{-\lambda\rho} \quad , \quad (4.66)$$

where A and B are constants. Second, if we substitute Eqs.(4.66) into the asymptotic relations (4.62), we obtain

$$-\frac{A}{B} = \frac{mc^2 + E}{\hbar c} = \left(\frac{mc^2 + E}{mc^2 - E} \right)^{1/2} = \left(\frac{1 + \epsilon}{1 - \epsilon} \right)^{1/2} \quad . \quad (4.67)$$

Eq.(4.67) indicates that for the usual binding of electrons in atoms, where $E = mc^2$, $F(\rho)$ is must larger than $G(\rho)$. These two functions can be referred to as "large" and "small" components, respectively.

4.5.2 Solutions for All Values of ρ : The above considerations of the asymptotic behaviors of $F(\rho)$ and $G(\rho)$ suggest that for all values of ρ we can write

$$F(\rho) = -(1 + \epsilon)^{1/2} \exp(-\lambda\rho) H^1(\rho) \quad , \quad (4.68)$$

$$G(\rho) = (1 - \epsilon)^{1/2} \exp(-\lambda\rho) H^2(\rho) \quad , \quad (4.69)$$

with the restrictions, which follows from Eq.(4.57) , that when one expands $H^1(\rho)$ and $H^2(\rho)$ in the powers of ρ , the first term in the expansions must be ρ^γ .

The equations in which $H^1(\rho)$ and $H^2(\rho)$ must satisfy can be obtained by substituting Eqs.(4.68) and (4.69) into Eqs.(4.53), the

* For the bound states, $0 < E < mc^2$, to which we shall devote our attention, we must choose the minus sign in the exponent in order to make the wave functions finite at infinity.

resulting equations are

$$\left(\frac{d}{d\bar{\rho}} + \frac{k}{\bar{\rho}} - \frac{1}{2} \right) H^1(\bar{\rho}) + \left(\frac{1}{2} + \frac{Z\alpha\hbar c}{mc^2\bar{\rho}(1+\epsilon)} \right) H^2(\bar{\rho}) = 0, \quad (4.70)$$

$$\left(\frac{d}{d\bar{\rho}} - \frac{k}{\bar{\rho}} - \frac{1}{2} \right) H^2(\bar{\rho}) + \left(\frac{1}{2} - \frac{Z\alpha\hbar c}{mc^2\bar{\rho}(1-\epsilon)} \right) H^1(\bar{\rho}) = 0, \quad (4.71)$$

where $\bar{\rho}$ is a dimensionless variable defined by

$$\bar{\rho} = 2\lambda\rho. \quad (4.72)$$

Instead of solving the pair of coupled first-order differential equations (4.70) and (4.71) for $H^1(\bar{\rho})$ and $H^2(\bar{\rho})$ simultaneously, we will try to find each function separately. The interrelationship between these two functions is then obtained by substituting them back into Eqs. (4.70) and (4.71). This method has been applied to the relativistic three dimensional hydrogen atom by Auvil and Brown (45), and by Waldenstrom (46).

4.5.3 The Large Component : The equation which involves only $H^1(\bar{\rho})$ can be found by first solving Eq. (4.70) for $H^2(\bar{\rho})$ in terms of $H^1(\bar{\rho})$ and then substituting the result into Eq. (4.71). After taking into account the relations (4.59) and

$$\frac{1}{\bar{\rho}^2(1+w\bar{\rho})} = \frac{1}{\bar{\rho}^2} - \frac{w}{\bar{\rho}(1+w\bar{\rho})}, \quad (4.73)$$

where w is a new dimensionless parameter defined by the relation

$$w = \frac{mc^2(1+\epsilon)}{2Z\alpha\hbar c\lambda}, \quad (4.74)$$

we get the equation for $H^1(\bar{\rho})$ in the form

$$\left(\frac{d^2}{d\bar{\rho}^2} + w\bar{\rho} \frac{d^2}{d\bar{\rho}^2} + \frac{1}{\bar{\rho}} \frac{d}{d\bar{\rho}} - \frac{d}{d\bar{\rho}} - w\bar{\rho} \frac{d}{d\bar{\rho}} - \frac{\gamma^2}{\bar{\rho}^2} - \frac{w\gamma^2}{\bar{\rho}} + \frac{(Z\alpha)^2 w}{\bar{\rho}} - \frac{k w}{\bar{\rho}} \right. \\ \left. - \frac{1}{4w\bar{\rho}} - \frac{1}{2\bar{\rho}} + (Z\alpha)^2 w^2 - \frac{1}{4} \right) H^1(\bar{\rho}) = 0 \quad (4.75)$$

This second order differential equation can be solved by using the power series method. Since the lowest power of $\bar{\rho}$ in the power series expansion of $H^1(\bar{\rho})$ must be γ , we write

$$H^1(\bar{\rho}) = \sum_{s=0}^{\infty} b_s \bar{\rho}^{s+\gamma} . \quad (4.76)$$

By (a) introducing the expression (4.76) into Eq.(4.75),

(b) collecting the terms of the same power of $\bar{\rho}$,

and (c) taking into account the relation

$$w(Z\alpha)^2 - \frac{1}{4w} = \frac{mc^2 Z\alpha \epsilon}{\hbar c \lambda} = \delta , \quad (4.77)$$

we obtain

$$\sum_{s=0}^{\infty} s(2\gamma + s) b_s \bar{\rho}^{s-2+\gamma} + \sum_{s=0}^{\infty} \left\{ \delta - \gamma - s + ws^2 + ws(2\gamma - 1) - w(\gamma + k) - \frac{1}{2} \right\} b_s \bar{\rho}^{s-1+\gamma} + \sum_{s=0}^{\infty} w(\delta - \gamma - s) b_s \bar{\rho}^{s+\gamma} = 0. \quad (4.78)$$

The coefficient of $\bar{\rho}^{\gamma-1}$ is

$$(2\gamma + 1)b_1 + \left\{ \delta - \gamma - w(\gamma + k) - \frac{1}{2} \right\} b_0 = 0 , \quad (4.79)$$

which gives the recursion relation between b_0 and b_1 ;

$$b_1 = \frac{2(\gamma - \delta) + (1 + 2w(\gamma + k))}{2(2\gamma + 1)} b_0 . \quad (4.80)$$

The general recursion relation can be obtained by equating the coefficient of $\bar{\rho}^{s+\gamma}$ to zero,

$$(s + 2)(2\gamma + s + 2)b_{s+2} + \left\{ \delta - \gamma - (s+1) + w(s + 1)^2 + w(s+1)(2\gamma - 1) - w(\gamma - k) - \frac{1}{2} \right\} b_{s+1} + w(\delta - \gamma - s)b_s = 0 ,$$

$$s = 0, 1, 2, 3, 4, \dots , \quad (4.81)$$



which is the three-term recursion relation, in contrast to the two-term relations normally encountered when dealing with the special functions of physics. For $s = 0$, we obtain

$$2(2\gamma + 2)b_2 + (\delta - \gamma - 1 + w + w(2\gamma - 1) - w(\gamma + k) - \frac{1}{2}b_1 + w(\delta - \gamma)b_0 = 0. \quad (4.82)$$

By using Eq.(4.80) we can solve, with the help of Eqs.(4.77) and (4.59), the above equation for b_2 either in terms of b_0 or b_1 ;

$$b_2 = \begin{cases} \frac{(\gamma - \delta + 1)(2(\gamma - \delta) + 2(1 + 2w(\gamma + k)))}{2(2\gamma + 1)(2\gamma + 2)} b_0, \\ \frac{(\gamma - \delta + 1)(2(\gamma - \delta) + 2(1 + 2w(\gamma + k)))}{2(2\gamma + 1)(2(\gamma - \delta) + (1 + 2w(\gamma + k)))} b_1. \end{cases} \quad (4.83)$$

For $s = 1$, Eq.(4.81) becomes

$$3(2\gamma + 3)b_3 + (\delta - \gamma - 2 + 4w + 2w(2\gamma - 1) - w(\gamma + k) - \frac{1}{2}b_2 + w(\delta - \gamma - 1)b_1 = 0, \quad (4.84)$$

which gives, by using Eqs.(4.80), (4.83) and (4.77),

$$b_3 = \begin{cases} \frac{(\gamma - \delta + 1)(\gamma - \delta + 2)(2(\gamma - \delta) + 3(1 + 3(1 + 2w(\gamma + k))))}{2(2\gamma + 1)(2\gamma + 2)(2\gamma + 3)3!} b_0, \\ \frac{(\gamma - \delta + 2)(2(\gamma - \delta) + 3(1 + 2w(\gamma + k)))}{3(2\gamma + 3)(2(\gamma - \delta) + 3(1 + 2w(\gamma + k)))} b_2. \end{cases} \quad (4.85)$$

In general, we can determine b_s/b_0 ($s > 1$) and b_{s+1}/b_s ($s \geq 0$) either by successive use of Eqs.(4.80) and (4.81) or by inspection of Eqs.(4.83) and (4.85). The results are

$$\frac{b_s}{b_0} = \frac{\left[\prod_{r=1}^{s-1} (\gamma - \delta - r) \right] \left\{ 2(\gamma - \delta) + s[1 + 2w(\gamma + k)] \right\}}{2 \left[\prod_{r=1}^s (2\gamma + s) \right] s!}; \quad s > 1, \quad (4.86)$$

and

$$\frac{b_{s+1}}{b_s} = \frac{(\gamma + \delta + s)(2(\gamma - \delta) + (s + 1)(1 + 2w(\gamma + k)))}{(s + 1)(2\gamma + s + 1)(2(\gamma - \delta) + s(1 + 2w(\gamma + k)))} ; s \geq 0, \quad (4.87)$$

where

$$\prod_{r=1}^n W(r) = W(1) \cdot W(2) \cdot W(3) \cdots W(n) . \quad (4.88)$$

Eqs.(4.80) and (4.86) show that $H^1(\bar{\rho})$ in Eq.(4.76) can be written as a sum of the two confluent hypergeometric functions multiplied by $\bar{\rho}$;

$$\begin{aligned} H^1(\bar{\rho}) &= \bar{\rho}^\gamma (b_0 + b_1 \bar{\rho} + b_2 \bar{\rho}^2 + b_3 \bar{\rho}^3 + \dots) \\ &= b_0 \bar{\rho}^\gamma \left[{}_1F_1(\gamma - \delta; 2\gamma + 1; \bar{\rho}) + \left\{ \frac{1 + 2w(\gamma + k)}{2(2\gamma + 1)} \right\} \bar{\rho} {}_1F_1(\gamma - \delta + 1; 2\gamma + 2; \bar{\rho}) \right], \end{aligned} \quad (4.89)$$

where

$${}_1F_1(a; c; x) = 1 + \frac{a}{c} x + \frac{a(a+1)}{c(c+1)} \frac{x^2}{2!} + \frac{a(a+1)(a+2)}{c(c+1)(c+2)} \frac{x^3}{3!} + \dots \quad (4.90)$$

is the confluent hypergeometric function. By using the recurrence relation

$$x {}_1F_1(a+1; c+1; x) = c \left\{ {}_1F_1(a+1; c; x) - {}_1F_1(a; c; x) \right\}, \quad (4.91)$$

which implies that

$$\bar{\rho} {}_1F_1(\gamma - \delta + 1; 2\gamma + 2; \bar{\rho}) = (2\gamma + 1) \left\{ {}_1F_1(\gamma - \delta + 1; 2\gamma + 1; \bar{\rho}) - {}_1F_1(\gamma - \delta; 2\gamma + 1; \bar{\rho}) \right\}, \quad (4.92)$$

Eq.(4.89) becomes

$$\begin{aligned} H^1(\bar{\rho}) &= b_0 \left[\frac{1 + 2w(\gamma + k)}{2} \right] \bar{\rho}^\gamma \left\{ {}_1F_1(\gamma - \delta + 1; 2\gamma + 1; \bar{\rho}) \right. \\ &\quad \left. - \left[\frac{2w(\gamma + k) - 1}{2w(\gamma + k) + 1} \right] {}_1F_1(\gamma - \delta; 2\gamma + 1; \bar{\rho}) \right\}. \end{aligned} \quad (4.93)$$

Thus, the large component of the radial wave function is , in terms of $\bar{\rho} = 2\lambda\rho$,

$$R^1(\bar{\rho}) = \left(\frac{\bar{\rho}}{2\lambda} \right)^{-\frac{1}{2}} F(\bar{\rho}) = -(1+\epsilon)^{\frac{1}{2}} \left(\frac{\bar{\rho}}{2\lambda} \right) \exp(-\frac{1}{2}\bar{\rho}) H^1(\bar{\rho}) . \quad (4.94)$$

4.5.4 Quantum Conditions : Let us examine the asymptotic behavior of $H^1(\bar{\rho})$. From Eq.(4.87), it follows that the coefficients of very high powers ($s \rightarrow \infty$) satisfy

$$\lim_{s \rightarrow \infty} \frac{b_{s+1}}{b_s} = \frac{1}{s+1} \quad (4.95)$$

which is the same as that of the series of $\exp(\bar{\rho})$. Thus, for large value $\bar{\rho}$, $H^1(\bar{\rho})$ behaves like $\bar{\rho}^\gamma \exp(\bar{\rho})$ and therefore $R^1(\bar{\rho})$ behaves like $\bar{\rho}^{\gamma - 1/2} \exp(\frac{1}{2} \bar{\rho})$, i.e., tends to infinity as $\bar{\rho} \rightarrow \infty$. The acceptable radial wave functions, which give a finite contribution to the probability density for all values of $\bar{\rho}$, can then be obtained only by interrupting the series in Eq.(4.93), that is, reducing them to polynomials.

By the definition (4.90), the confluent hypergeometric function will reduce to a polynomials of degree \bar{n} when $a = -\bar{n}$, where \bar{n} is any nonnegative integer or zero. Hence, the function $H^1(\bar{\rho})$ will reduce to a polynomials of degree $(\gamma + \bar{n})$ when

$$\gamma - \delta = -\bar{n} \quad , \quad \bar{n} = 0, 1, 2, 3, \dots \quad (4.96)$$

This is the general 'quantum condition' for the relativistic two dimensional hydrogen atom.

For the cases in which $\bar{n} = 0$, the series of ${}_1F_1(\gamma - \delta + 1; 2\gamma + 1; \bar{\rho})$ does not terminate and hence tend to infinity as $\bar{\rho} \rightarrow \infty$:

$${}_1F_1(\gamma - \delta + 1; 2\gamma + 1; \bar{\rho}) \xrightarrow{\bar{n} = 0} {}_1F_1(1, 2\gamma + 1; \bar{\rho}) = 1 + \frac{\bar{\rho}}{(2\gamma + 1)} + \frac{\bar{\rho}^2}{2!(2\gamma + 1)(2\gamma + 2)} + \dots \quad (4.97)$$

Thus, in order to get an acceptable radial functions for the cases $\bar{n} = 0$, we must add the condition

$$1 + 2w(\gamma + k) = 2w\left(\frac{1}{2w} + \gamma + k\right) = 0 . \quad (4.98)$$

Since, for $\bar{n} = 0$,

$$\frac{1}{2w} + \gamma = \frac{1}{2w} + \delta = |k| , \quad (4.99)$$

Eq.(4.98) becomes

$$2w(|k| + k) = 0 . \quad (4.100)$$

This means that the acceptable radial functions for $\bar{n} = 0$ all belong to the class for which the values of k are negative, $k = -|k|$, where as, for $\bar{n} \neq 0$, both negative and positive values of k are possible.

4.5.5 Energy Eigenvalues : The allowed values of the energy of the electron, in the unit of the rest mass mc^2 , can be obtained from the quantum condition (4.96) by inserting the expression for δ , Eq.(4.77), and solving for ϵ ; the result is

$$\epsilon = \left\{ 1 + \frac{(Z\alpha)^2}{(\gamma + \bar{n})^2} \right\}^{-1/2} = \epsilon_{\bar{n}k} \quad (4.101)$$

where the subscripts \bar{n} and k are added to ϵ to denote its dependence on the quantum numbers \bar{n} and k .

By defining a new quantum number n ,

$$n = \bar{n} + |k| + \frac{1}{2} = 1, 2, 3, \dots , \quad (4.102)$$

(since $\bar{n} = 0, 1, 2, \dots$, and $|k| = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$) and using Eq.(4.59) Eq. (4.101) becomes

$$\epsilon = \left\{ 1 + \left[\frac{Z\alpha}{n - |k| - \frac{1}{2} + \sqrt{(k^2 - (Z\alpha)^2)}} \right]^2 \right\}^{-1/2} = \epsilon_{nk} . \quad (4.103)$$

The parameters λ and w are, by the definitions (4.64) and (4.74), depend on the energy eigenvalue ϵ and therefore on the quantum numbers n and k . To indicate their dependence on n and k , we may write

$$\lambda = \lambda_{nk} = \frac{mc^2}{\hbar c} (1 - \epsilon_{nk}^2)^{1/2}, \quad (4.104)$$

$$w = w_{nk} = \frac{mc^2 (1 + \epsilon_{nk})}{2Z\alpha\hbar c \lambda_{nk}}. \quad (4.105)$$

However, it is convenient to write them without the subscripts.

As in the case of the three dimensional hydrogen atom (22), it is useful to introduce a quantity N_{nk} defined by the relation

$$1 - \epsilon_{nk}^2 = \frac{(Z\alpha)^2}{N_{nk}^2}, \quad (4.106)$$

so that

$$\begin{aligned} N_{nk} &= \left[\left\{ (n - |k| - 1/2) + \sqrt{k^2 + (Z\alpha)^2} \right\}^2 + (Z\alpha)^2 \right]^{1/2} \\ &= \left\{ (\bar{n})^2 + 2\bar{n} + k^2 \right\}^{1/2} = N_{nk}^- \end{aligned} \quad (4.107)$$

In terms of this quantity, Eq.(4.103) can be written as

$$\epsilon_{nk} = \left\{ 1 - \left(\frac{Z\alpha}{N_{nk}} \right)^2 \right\}^{1/2} = \left(\frac{\bar{n} + \gamma}{N_{nk}} \right). \quad (4.108)$$

Let us return to the radial function $H^1(\bar{0})$. Since

$$\frac{1}{2w} = \frac{Z\alpha\hbar c \lambda}{mc^2(1 + \epsilon)} = \frac{Z\alpha\hbar c \lambda (1 - \epsilon)}{mc^2(1 - \epsilon^2)} = N_{nk} - \bar{n} - \gamma, \quad (4.109)$$

then, after taking into account the relation

$$N_{nk}^2 - k^2 = (\bar{n})^2 + 2\bar{n}\gamma, \quad (4.110)$$

it follows that

$$\begin{aligned}
\frac{2w(\gamma + k) - 1}{2w(\gamma + k) + 1} &= \frac{\gamma + k - \frac{1}{2w}}{\gamma + k + \frac{1}{2w}} = \frac{2\gamma + k - N_{nk} + \bar{n}}{k + N_{nk} - \bar{n}} \\
&= \frac{(N_{nk} - k) \left\{ \left[\frac{2\gamma + \bar{n}}{N_{nk} - k} \right] - 1 \right\}}{\bar{n} \left\{ \left[\frac{N_{nk} + k}{\bar{n}} \right] - 1 \right\}} \\
&= \left(\frac{N_{nk} - k}{\bar{n}} \right) \quad . \quad (4.111)
\end{aligned}$$

With this relation and Eq.(4.96), we can write Eq.(4.93) as

$$\begin{aligned}
H_{nk}^1(\bar{\rho}) &= c_{nk}^1 \bar{\rho}^{\gamma_k} \left\{ \bar{n} {}_1F_1(-\bar{n} + 1; 2\gamma_k + 1; \bar{\rho}) \right. \\
&\quad \left. - (N_{nk} - k) {}_1F_1(-\bar{n}; 2\gamma_k + 1; \bar{\rho}) \right\} \quad (4.112)
\end{aligned}$$

where

$$c_{nk}^1 = \frac{b_0}{2} \left\{ \frac{1 + 2w_{nk}(\gamma_k + k)}{\bar{n}} \right\} \quad (4.113)$$

is a constant multiplying factor to be determined from the normalization condition of the wave function. The large component of the radial wave function then takes the form

$$\begin{aligned}
R_{nk}^1(\bar{\rho}) &= - 2\lambda_{nk} (1 + \epsilon_{nk})^{1/2} c_{nk}^1 \exp\left(-\frac{\bar{\rho}}{2}\right) (\bar{\rho})^{\gamma_k - 1/2} \\
&\quad \left\{ \bar{n} {}_1F_1(-\bar{n} + 1; 2\gamma_k + 1; \bar{\rho}) - (N_{nk} - k) {}_1F_1(-\bar{n}; 2\gamma_k + 1; \bar{\rho}) \right\}. \quad (4.114)
\end{aligned}$$

4.5.6 The Small Component : In a similar manner, the corresponding expressions for $H^2(\bar{\rho})$ can be obtained by, first, deriving from Eqs.(4.70) and (4.71) the equation which involves $H^2(\bar{\rho})$ only, then solving for $H^2(\bar{\rho})$ by means of the power series method. By

(a) solving Eq.(4.71) for $H^1(\bar{\rho})$ in terms of $H^2(\bar{\rho})$,

(b) substituting the result into Eq.(4.70),

(c) introducing a new dimensionless parameter \bar{w} and a new quantum number \bar{k} ;

$$\bar{w} = - \frac{mc^2(1 - \epsilon)}{2Z\alpha\hbar c\lambda} \quad , \quad (4.115)$$

$$\bar{k} = - k \quad , \quad (4.116)$$

and (d) taking into account the relations

$$\gamma^2 = k^2 - (Z\alpha)^2 = \bar{k}^2 - (Z\alpha)^2 \quad (4.117)$$

and

$$\frac{1}{(\bar{\rho})^2(1 + \bar{w}\bar{\rho})} = \frac{1}{(\bar{\rho})^2} - \frac{\bar{w}}{\bar{\rho}(1 + \bar{w}\bar{\rho})} \quad (4.118)$$

we obtain the equation for $H^2(\bar{\rho})$ which is identical in form with that for $H^1(\bar{\rho})$, Eq.(4.75), except that w and k are now replaced by \bar{w} and \bar{k} , respectively, namely,

$$\left[\frac{d^2}{d\bar{\rho}^2} + w\rho \frac{d^2}{d\bar{\rho}^2} + \frac{1}{\bar{\rho}} \frac{d}{d\bar{\rho}} - \frac{d}{d\bar{\rho}} - \frac{\bar{w}}{\bar{\rho}} \frac{d}{d\bar{\rho}} - \frac{\gamma^2}{\bar{\rho}^2} + \frac{(Z\alpha)^2 \bar{w}}{\bar{\rho}} - \frac{\bar{k}\bar{w}}{\bar{\rho}} - \frac{1}{4\bar{w}\bar{\rho}} - \frac{1}{2\bar{\rho}} + (Z\alpha)^2 \bar{w}^2 - \frac{1}{4} \right] H^2(\bar{\rho}) = 0 \quad . \quad (4.119)$$

In the case of the large component, the results of solving Eq.(4.75) by the series method, i.e., Eqs.(4.86), (4.87) and (4.93), are obtained by using the algebraic relation (4.77). Since

$$\bar{w}(Z\alpha)^2 - \frac{1}{4\bar{w}} = \frac{mc^2 Z\alpha\epsilon}{\hbar c\lambda} = \delta \quad , \quad (4.120)$$

that is, \bar{w} obeys the same algebraic relation as w , we can conclude that by substituting into Eq.(4.119) the expression

$$H^2(\bar{\rho}) = \sum_{s=0}^{\infty} \bar{b}_s \bar{\rho}^{s+\gamma} \quad (4.121)$$

we get (a) the recursion relations :

$$\frac{\bar{b}_s}{\bar{b}_0} = \frac{\left[\prod_{r=1}^{s-1} (\gamma - \delta - r) \right] \left\{ 2(\gamma - \delta) + s(1 + 2\bar{w}(\gamma + \bar{k})) \right\}}{2 \left[\prod_{r=1}^s (2\gamma + r) \right] s!}, \quad s > 1, \quad (4.122)$$

$$\frac{\bar{b}_{s+1}}{\bar{b}_s} = \frac{(\gamma - \delta + s) [2(\gamma - \delta) + (s+1)(1 + 2\bar{w}(\gamma + \bar{k}))]}{(s+1)(2\gamma + s+1) [2(\gamma - \delta) + s(1 + 2\bar{w}(\gamma + \bar{k}))]}, \quad s \geq 0, \quad (4.123)$$

and (b) the expression for $H^2(\bar{\rho})$:

$$H^2(\bar{\rho}) = \bar{b}_0 \left[\frac{1 + 2\bar{w}(\gamma + \bar{k})}{2} \right] \bar{\rho}^{-\gamma} \left\{ {}_1F_1(\gamma - \delta + 1; 2\gamma + 1; \bar{\rho}) - \left[\frac{2\bar{w}(\gamma + \bar{k}) - 1}{2\bar{w}(\gamma + \bar{k}) + 1} \right] {}_1F_1(\gamma - \delta; 2\gamma + 1; \bar{\rho}) \right\}. \quad (4.124)$$

The small component of the radial wave function is then

$$R^4(\bar{\rho}) = [2\lambda(1 - \epsilon)]^{1/2} (\bar{\rho})^{-1/2} \exp(-1/2 \bar{\rho}) H^2(\bar{\rho}). \quad (4.125)$$

Similar to the case of the large component, the requirement that the small component must give a finite contribution to the probability density leads to the general 'quantum condition'

$$\gamma - \delta = -\bar{n}, \quad \bar{n} = 0, 1, 2, 3, \dots, \quad (4.96)$$

and the additional condition for $\bar{n} = 0$

$$1 + 2\bar{w}(\gamma + \bar{k}) = 2\bar{w} \left(\frac{1}{2\bar{w}} + \gamma - k \right) = 0. \quad (4.126)$$

Since

$$\frac{1}{2\bar{w}} = -\frac{Z\alpha\hbar c\lambda}{mc^2(1-\epsilon)} = -\frac{Z\alpha\hbar c\lambda(1+\epsilon)}{mc^2(1-\epsilon^2)} = -(N_{nk} + \bar{n} + \gamma), \quad (4.127)$$

Eq.(4.126) reduces to, with the help of Eq.(4.107),

$$k = -N_{nk} = -|k|; \quad \bar{n} = 0 \quad (4.128)$$

that is, for $\bar{n} = 0$ the acceptable solutions must belong to the class for which the values of k are negative.

By using the quantum condition (4.96) and the relation

$$\frac{2\bar{w}(\gamma + \bar{k}) - 1}{2\bar{w}(\gamma + \bar{k}) + 1} = -\left\{ \frac{N_{nk} - k}{\bar{n}} \right\}, \quad (4.129)$$

the expressions for $H^2(\rho)$ and $R^4(\rho)$, Eqs.(4.124) and (4.125), become

$$H_{nk}^2(\rho) = c_{nk}^2 \bar{\rho}^{\gamma_k} \left\{ \bar{n} {}_1F_1(-\bar{n} + 1; 2\gamma_k + 1; \bar{\rho}) + (N_{nk} - k) {}_1F_1(-\bar{n}; 2\gamma_k + 1; \bar{\rho}) \right\}, \quad (4.130)$$

and

$$R_{nk}^4(\rho) = [2\lambda_{nk}(1 - \epsilon_{nk})] c_{nk}^2 \exp\left(-\frac{\bar{\rho}}{2}\right) (\bar{\rho})^{\gamma_k - \frac{1}{2}} \left\{ \bar{n} {}_1F_1(-\bar{n} + 1; 2\gamma_k + 1; \bar{\rho}) + (N_{nk} - k) {}_1F_1(-\bar{n}; 2\gamma_k + 1; \bar{\rho}) \right\}, \quad (4.131)$$

where

$$c_{nk}^2 = \frac{\bar{b}_0}{2} \left\{ \frac{1 + 2w_{nk}(\gamma_k - k)}{\bar{n}} \right\} \quad (4.132)$$

is a constant multiplying factor to be determined from the normalization condition.

4.5.7 Relation Between c_{nk}^1 and c_{nk}^2 : From the forms of $H_{nk}^1(\bar{\rho})$ and $H_{nk}^2(\bar{\rho})$ it can be seen that the relation between them is now reduced to the relation between c_{nk}^1 and c_{nk}^2 . To find the relation between these two constant multiplying factors, we first substitute into Eqs.(4.70) and (4.71) the expansions

$$H^1(\bar{\rho}) = \sum_{s=0}^{\infty} B_s \bar{\rho}^{s+\gamma} \quad \text{and} \quad H^2(\bar{\rho}) = \sum_{s=0}^{\infty} \bar{B}_s \bar{\rho}^{s+\gamma}, \quad (4.133)$$

then equate the coefficients of $\bar{\rho}^{s+1+\gamma}$ to zero. The results are, with the help of Eqs.(4.109) and (4.127),

$$(s+k+\gamma)B_s - \frac{1}{2} B_{s-1} + (N_{nk} - \bar{n} - \gamma)\bar{B}_s + \frac{1}{2} \bar{B}_{s-1} = 0, \quad (4.134)$$

$$-(N_{nk} + \bar{n} + \gamma)B_s + \frac{1}{2} B_{s-1} + (s-k+\gamma)\bar{B}_s - \frac{1}{2} \bar{B}_{s-1} = 0, \quad (4.135)$$

where $B_{-1} = \bar{B}_{-1} = 0$. For $s = 0$, Eqs.(4.134) and(4.135) reduce to

$$(\gamma+k)B_0 + (N_{nk} - \bar{n} - \gamma)\bar{B}_0 = 0, \quad (4.136)$$

$$-(N_{nk} + \bar{n} + \gamma)B_0 + (\gamma-k)\bar{B}_0 = 0, \quad (4.137)$$

respectively. Adding the last two equations, we get

$$(k - N_{nk} - \bar{n})B_0 + (N_{nk} - \bar{n} - k)\bar{B}_0 = 0. \quad (4.138)$$

A comparison of Eqs.(4.112) and (4.131) with the two expansions in Eq. (4.133) leads to the relations

$$B_0 = c_{nk}^1 (\bar{n} - N_{nk} + k) \quad \text{and} \quad \bar{B}_0 = c_{nk}^2 (\bar{n} + N_{nk} - k). \quad (4.139)$$

Substituting these two relations into Eq.(4.138), we obtain

$$(\bar{n} - N_{nk} + k)(k - N_{nk} - \bar{n})c_{nk}^1 + (\bar{n} + N_{nk} - k)(N_{nk} - \bar{n} - k)c_{nk}^2 = 0,$$

that is,

$$c_{nk}^1 = -c_{nk}^2 = c_{nk}. \quad (4.140)$$

4.6 NORMALIZATION OF THE WAVE FUNCTIONS.

In the case of the two dimensional hydrogen atom, the electron can move only in a plane, the normalization condition then takes the form, in the plane polar coordinates (ρ, ϕ) ,

$$\int_0^{\infty} \int_0^{2\pi} [U(\rho, \phi)]^* U(\rho, \phi) d\phi \rho d\rho = 1. \quad (4.141)$$

From the forms of the wave functions, Eqs.(4.40), (4.41) and (4.51), it follows that for both $U_{njk}^A(\rho, \phi)$ and $U_{njk}^B(\rho, \phi)$ Eq.(4.141) reduces to

$$\int_0^{\infty} (|R_{nk}^1(\rho)|^2 + |R_{nk}^4(\rho)|^2) \rho d\rho = 1, \quad (4.142)$$

or, in terms of the dimensionless variable $\bar{\rho} = 2\lambda_{nk}\rho$,

$$(2\lambda_{nk})^{-2} \int_0^{\infty} (|R_{nk}^1(\bar{\rho})|^2 + |R_{nk}^4(\bar{\rho})|^2) \bar{\rho} d\bar{\rho} = 1. \quad (4.143)$$

Using Eqs.(4.114), (4.131) and (4.140), Eq.(4.143) becomes

$$\begin{aligned} & \frac{(c_{nk})^2}{2\lambda_{nk}} \int_0^{\infty} \left\{ 2(\bar{n})^2 [{}_1F_1(-\bar{n}+1; 2\gamma_k+1; \bar{\rho})]^2 - \right. \\ & \quad \left. 2\epsilon_{nk} \bar{n}(N_{nk}-k) {}_1F_1(-\bar{n}; 2\gamma_k+1; \bar{\rho}) {}_1F_1(-\bar{n}+1; 2\gamma_k+1; \bar{\rho}) + \right. \\ & \quad \left. 2(N_{nk}-k)^2 [{}_1F_1(-\bar{n}; 2\gamma_k+1; \bar{\rho})]^2 \right\} \exp(-\bar{\rho}) (\bar{\rho})^{2\gamma_k} d\bar{\rho} \\ & = 1. \end{aligned} \quad (4.144)$$

By using the relation, see Appendix A,

$$\begin{aligned} & \int_0^{\infty} z^c \exp(-z) {}_1F_1(-m; c+1; z) {}_1F_1(-n; c+1; z) dz \\ & = \frac{[\Gamma(c+1)]^2 n!}{\Gamma(n+c+1)} \delta_{mn}, \end{aligned} \quad (4.145)$$

where m and n are positive integers or zero; c may be any complex

number; δ_{mn} is the Kronecker symbol

$$\delta_{mn} = \begin{cases} 0 & \text{for } m \neq n \\ 1 & \text{for } m = n \end{cases} ;$$

and $\Gamma(s)$ is the gamma function

$$\Gamma(s) = \int_0^{\infty} u^{s-1} e^{-u} du, \quad \Gamma(s+1) = s\Gamma(s), \quad (4.146)$$

which implies the following relations

$$\begin{aligned} \int_0^{\infty} [{}_1F_1(-\bar{n}+1; 2\gamma_k+1; \bar{\rho})]^2 \exp(-\bar{\rho}) \bar{\rho}^{2\gamma_k} d\bar{\rho} &= \frac{[\Gamma(2\gamma_k+1)]^2 (\bar{n}-1)!}{\Gamma(\bar{n}+2\gamma_k)} \\ &= \frac{[\Gamma(2\gamma_k+1)]^2 \bar{n}! \Gamma(\bar{n}+2\gamma_k)}{\bar{n} \Gamma(\bar{n}+2\gamma_k+1)}, \end{aligned} \quad (4.147)$$

$$\int_0^{\infty} {}_1F_1(-\bar{n}+1; 2\gamma_k+1; \bar{\rho}) {}_1F_1(-\bar{n}; 2\gamma_k+1; \bar{\rho}) \exp(-\bar{\rho}) \bar{\rho}^{2\gamma_k} d\bar{\rho} = 0, \quad (4.148)$$

and

$$\int_0^{\infty} [{}_1F_1(-\bar{n}; 2\gamma_k+1; \bar{\rho})]^2 \exp(-\bar{\rho}) \bar{\rho}^{2\gamma_k} d\bar{\rho} = \frac{[\Gamma(2\gamma_k+1)]^2 \bar{n}!}{\Gamma(\bar{n}+2\gamma_k+1)}, \quad (4.149)$$

Eq.(4.144) becomes, with the help of Eq.(4.110),

$$\frac{(c_{nk})^2}{2\lambda_{nk}} = \frac{4N_{nk} (N_{nk}-k) [\Gamma(2\gamma_k+1)]^2 \bar{n}!}{\Gamma(\bar{n}+2\gamma_k+1)} = 1. \quad (4.150)$$

That is,

$$c_{nk} = \left\{ \frac{2\lambda_{nk} \Gamma(\bar{n}+2\gamma_k+1)}{4N_{nk} (N_{nk}-k) [\Gamma(2\gamma_k+1)]^2 \bar{n}!} \right\}^{1/2}. \quad (4.151)$$

Hence, the normalized wave functions of the relativistic two dimensional hydrogen atom which correspond to the energy eigenvalue ϵ_{nk} , Eq.(4.103), are

$$U_{njk}^A(\rho, \phi) = \begin{bmatrix} R_{nk}^1(\rho) \phi_j^1(\phi) \\ 0 \\ 0 \\ -iR_{nk}^4(\rho) \phi_j^2(\phi) \end{bmatrix}, \quad (4.152)$$

and

$$U_{njk}^B(\rho, \phi) = \begin{bmatrix} 0 \\ R_{nk}^1(\rho) \phi_j^2(\phi) \\ -iR_{nk}^4(\rho) \phi_j^1(\phi) \\ 0 \end{bmatrix}, \quad (4.153)$$

where

$$R_{nk}^1(\rho) = - \left\{ \frac{(\lambda_{nk})^2 \Gamma(\bar{n} + 2\gamma_k + 1)}{N_{nk} (N_{nk} - k) [\Gamma(2\gamma_k + 1)]^2 \bar{n}!} \right\}^{\frac{1}{2}} (2\lambda_{nk}\rho)^{\gamma_k - \frac{1}{2}} \exp(-\lambda_{nk}\rho) \\ (1 + \epsilon_{nk})^{\frac{1}{2}} \left\{ \bar{n} {}_1F_1(-\bar{n} + 1; 2\gamma_k + 1; 2\lambda_{nk}\rho) - (N_{nk} - k) {}_1F_1(-\bar{n}; 2\gamma_k + 1; 2\lambda_{nk}\rho) \right\}, \quad (4.154)$$

$$R_{nk}^4(\rho) = - \left\{ \frac{(\lambda_{nk})^2 \Gamma(\bar{n} + 2\gamma_k + 1)}{N_{nk} (N_{nk} - k) [\Gamma(2\gamma_k + 1)]^2 \bar{n}!} \right\}^{\frac{1}{2}} (2\lambda_{nk}\rho)^{\gamma_k - \frac{1}{2}} \exp(-\lambda_{nk}\rho) \\ (1 - \epsilon_{nk})^{\frac{1}{2}} \left\{ \bar{n} {}_1F_1(-\bar{n} + 1; 2\gamma_k + 1; 2\lambda_{nk}\rho) + (N_{nk} - k) {}_1F_1(-\bar{n}; 2\gamma_k + 1; 2\lambda_{nk}\rho) \right\}, \quad (4.155)$$

$$\phi_j^1(\phi) = \frac{1}{\sqrt{(2\pi)}} \exp(i(j - \frac{1}{2})\phi), \quad (4.42)$$

and

$$\phi_j^2(\phi) = \frac{1}{\sqrt{(2\pi)}} \exp(i(j + \frac{1}{2})\phi). \quad (4.43)$$

4.7 NONRELATIVISTIC LIMIT AND GRAPHIC REPRESENTATION OF THE RELATIVISTIC NORMALIZED RADIAL FUNCTIONS.

In the nonrelativistic limit, $(Z\alpha)^2$ is neglected compared to unity, so that $\gamma_k = k$ and ϵ_{nk} is set equal to 1. Then, from Eqs.(4.154) and (4.155), only the large components survive. For $U_{njk}^A(\rho, \phi)$ the large components have the angular factors

$$\exp(i(j - \frac{1}{2})\phi) , \quad (4.156)$$

indicating that the eigenvalues of the orbital angular momentum are

$$l = j - \frac{1}{2} , \quad (4.157)$$

while for $U_{njk}^B(\rho, \phi)$ the large components have the angular factors

$$\exp(i(j + \frac{1}{2})\phi) , \quad (4.158)$$

for which

$$l = j + \frac{1}{2} . \quad (4.159)$$

Thus, in addition to the quantum numbers n , j and k , we may assign to each $U_{njk}(\rho, \phi)$ the quantum number l such that

$$l = \begin{cases} j - \frac{1}{2} & \text{for } k = -j \\ j + \frac{1}{2} & \text{for } k = j \end{cases} . \quad (4.160)$$

Comparing with the nonrelativistic case, Chapter III, it can be concluded that the eigenfunctions belonging to the first set, $U_{njk}^A(\rho, \phi)$, are correspond to the spin-up states, where as those belonging to the second set, $U_{njk}^B(\rho, \phi)$, are correspond to the spin-down states.

Table 4.1 gives the possible values of n , j , k and l for $n = 1, 2, 3, 4$.

TABLE 4.1 The possible values of \bar{n} , k , j , l and the spectroscopic notations for the relativistic states with $n = 1, 2, 3, 4$.

n	\bar{n}	$ k $	k	j	l	Spectroscopic Notation
1	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$1S_{0, \frac{1}{2}}$
				$-\frac{1}{2}$	0	$1S_{0, -\frac{1}{2}}$
2	1	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$2S_{0, \frac{1}{2}}$
				$-\frac{1}{2}$	0	$2S_{0, -\frac{1}{2}}$
				$\frac{1}{2}$	$-\frac{1}{2}$	$2P_{-1, \frac{1}{2}}$
	0	$\frac{3}{2}$	$-\frac{3}{2}$	$\frac{1}{2}$	1	$2P_{1, -\frac{1}{2}}$
				$\frac{3}{2}$	1	$2P_{1, \frac{1}{2}}$
				$-\frac{3}{2}$	-1	$2P_{-1, -\frac{1}{2}}$
3	2	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$3S_{0, \frac{1}{2}}$
				$-\frac{1}{2}$	0	$3S_{0, -\frac{1}{2}}$
				$\frac{1}{2}$	-1	$3P_{-1, \frac{1}{2}}$
				$\frac{1}{2}$	1	$3P_{1, -\frac{1}{2}}$
	1	$\frac{3}{2}$	$-\frac{3}{2}$	$\frac{1}{2}$	1	$3P_{1, \frac{1}{2}}$
				$\frac{3}{2}$	-1	$3P_{-1, -\frac{1}{2}}$
				$\frac{3}{2}$	-2	$3D_{-2, \frac{1}{2}}$
				$\frac{3}{2}$	2	$3D_{2, -\frac{1}{2}}$
0	$\frac{5}{2}$	$-\frac{5}{2}$	$\frac{5}{2}$	2	$3D_{2, \frac{1}{2}}$	
			$-\frac{5}{2}$	-2	$3D_{-2, -\frac{1}{2}}$	

TABLE 4.1 (continued)

n	\bar{n}	$ k $	k	j	l	Spectroscopic Notation			
4	3	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$4S_{0, \frac{1}{2}}$			
				$-\frac{1}{2}$	0	$4S_{0, -\frac{1}{2}}$			
	2	$\frac{3}{2}$	$-\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	-1	$4P_{-1, \frac{1}{2}}$		
				$\frac{1}{2}$	$\frac{1}{2}$	1	$4P_{1, -\frac{1}{2}}$		
				$\frac{3}{2}$	$-\frac{3}{2}$	1	$4P_{1, \frac{1}{2}}$		
				$-\frac{3}{2}$	-1	$4P_{-1, -\frac{1}{2}}$			
		1	$\frac{5}{2}$	$-\frac{5}{2}$	$\frac{3}{2}$	$-\frac{3}{2}$	-2	$4D_{-2, \frac{1}{2}}$	
					$\frac{3}{2}$	$\frac{3}{2}$	2	$4D_{2, -\frac{1}{2}}$	
					$\frac{5}{2}$	$-\frac{5}{2}$	2	$4D_{2, \frac{1}{2}}$	
			0	$\frac{7}{2}$	$-\frac{7}{2}$	$-\frac{5}{2}$	$-\frac{5}{2}$	-2	$4D_{-2, -\frac{1}{2}}$
						$\frac{5}{2}$	$-\frac{5}{2}$	-3	$4F_{-3, \frac{1}{2}}$
						$\frac{5}{2}$	$\frac{5}{2}$	3	$4F_{3, -\frac{1}{2}}$
	0	$\frac{7}{2}$	$-\frac{7}{2}$	$\frac{7}{2}$	$\frac{7}{2}$	3	$4F_{3, \frac{1}{2}}$		
				$-\frac{7}{2}$	-3	$4F_{-3, -\frac{1}{2}}$			

In order to compare the relativistic states with the non-relativistic states obtained in Chapter III, it is convenient to assign to each state the spectroscopic notation nX_{l,m_s} , where X is a capital letter representing the value of $|l|$ according to the code

$ l $	0	1	2	3	4 ...
symbol	S	P	D	F	G ...

and m_s is equal to $-\frac{1}{2}$ or $\frac{1}{2}$ depending on the spin state, i.e., $-\frac{1}{2}$ for the spin-down state and $\frac{1}{2}$ for the spin-up state. It can be easily seen from Table 4.1 that for each nonrelativistic state identified by the spectroscopic notation nX_l , there are two relativistic corresponding states $nX_{l,\frac{1}{2}}$ and $nX_{l,-\frac{1}{2}}$, which arise from the two possible orientation of the electron spin.

The radial functions for the relativistic states which correspond to the same nonrelativistic state are identical for $l = 0$ and are different for $l \neq 0$. Moreover, the relativistic states with the same values of n and k have the same radial function.

However, according to the correspondence principle, in the nonrelativistic limit the wave function for the relativistic state must reduce to that for the corresponding nonrelativistic state. Since in this limit the angular parts of the relativistic and non-relativistic wave functions are obviously the same, and the radial function of the small component of the relativistic wave function is already shown to be vanish, the remaining is to show that in the nonrelativistic limit the radial function of the large component reduces to the nonrelativistic radial function. To demonstrate this we must first notice that, as can be seen from Table 4.1, for the

states with negative k , the values of l which correspond to spin-up and spin-down states are

$$l = 0, 1, 2, 3, \dots,$$

and

$$l = 0, -1, -2, -3, \dots,$$

respectively, so that k and $|k|$ can be written in terms of $|l|$ as

$$k = -(|l| + \frac{1}{2}) \quad , \quad \text{negative } k \quad , \quad (4.161a)$$

$$|k| = |l| + \frac{1}{2} \quad , \quad \text{negative } k \quad . \quad (4.161b)$$

Where as, for the state with positive k ,

$$k = |l| - \frac{1}{2} \quad , \quad \text{positive } k \quad , \quad (4.162a)$$

$$|k| = |l| - \frac{1}{2} \quad , \quad \text{positive } k \quad . \quad (4.162b)$$

Thus, in the nonrelativistic limit ($c \rightarrow \infty$ or/and $\alpha \rightarrow 0$), we have

$$\gamma_k \xrightarrow{\alpha \rightarrow 0} |k| = \begin{cases} |l| + \frac{1}{2} & ; \text{negative } k \\ |l| - \frac{1}{2} & ; \text{positive } k \end{cases} \quad , \quad (4.163a)$$

$$\bar{n} = n - |k| - \frac{1}{2} = \begin{cases} n - |l| - 1 & ; \text{negative } k \\ n - |l| & ; \text{positive } k \end{cases} \quad , \quad (4.163b)$$

$$N_{nk} = [(\bar{n})^2 + 2\bar{n}\gamma_k + k^2]^{\frac{1}{2}} \xrightarrow{\alpha \rightarrow 0} n - \frac{1}{2} \quad , \quad (4.163c)$$

$$\epsilon_{nk} = \frac{\bar{n} + \gamma_k}{N_{nk}} \xrightarrow{\alpha \rightarrow 0} 1 \quad , \quad (4.163d)$$

$$\begin{aligned} \lambda_{nk} &= \frac{mc}{\hbar} (1 - (\epsilon_{nk})^2)^{\frac{1}{2}} = \frac{mcZ\alpha}{\hbar N_{nk}} = \frac{mZe^2}{\hbar^2 N_{nk}} \\ &\xrightarrow{\alpha \rightarrow 0} \frac{mZe^2}{\hbar^2 (n - \frac{1}{2})} = \frac{\beta}{2} \end{aligned} \quad (4.163e)$$

Thus

$$R_{nk}^1(\rho) \rightarrow \left\{ \begin{array}{l} - \left\{ \frac{\beta^2 \Gamma(n+|l|+1)}{4(n-\frac{1}{2})(n+|l|) [\Gamma(2|l|+2)]^2 \Gamma(n-|l|)} \right\}^{\frac{1}{2}} (\beta\rho)^{|l|} \exp(-\frac{\beta\rho}{2}) \\ \quad \sqrt{2} \left[(n-|l|-1) {}_1F_1(-n+|l|+2; 2|l|+2; \beta\rho) - \right. \\ \quad \left. - (n+|l|) {}_1F_1(-n+|l|+1; 2|l|+2; \beta\rho) \right]; \text{ negative } k, \\ \hspace{15em} (4.164a) \\ - \left\{ \frac{\beta^2 \Gamma(n+|l|)}{4(n-\frac{1}{2})(n+|l|) [\Gamma(2|l|)]^2 \Gamma(n-|l|+1)} \right\}^{\frac{1}{2}} (\beta\rho)^{|l|-1} \exp(-\frac{\beta\rho}{2}) \\ \quad \sqrt{2} \left[(n-|l|) {}_1F_1(-n+|l|+1; 2|l|; \beta\rho) \right. \\ \quad \left. - (n-|l|) {}_1F_1(-n+|l|; 2|l|; \beta\rho) \right]; \text{ positive } k. \\ \hspace{15em} (4.164b) \end{array} \right.$$

By applying to the cases of negative and positive k the recurrence relations (47)

$$(1+a-b) {}_1F_1(a; b; z) - a {}_1F_1(a+1; b; z) = (1-b) {}_1F_1(a; b-1; z) \quad (4.165a)$$

and

$${}_1F_1(a; b; z) - {}_1F_1(a-1; b; z) = \left(\frac{z}{b}\right) {}_1F_1(a; b+1; z), \quad (4.165b)$$

respectively, we obtain

$$R_{nk}^1(\rho) \xrightarrow[\rho \rightarrow \infty]{\alpha \rightarrow 0} \begin{cases} R_{nl}(\rho) & \text{for negative } k \\ -R_{nl}(\rho) & \text{for positive } k \end{cases} \quad \begin{array}{l} (4.166a) \\ (4.166b) \end{array}$$

$R_{nl}(\rho)$ = nonrelativistic radial function

which demonstrate the validity of the correspondence principle, since the negative sign in Eq.(4.166b) has no effect on the values of the physical observable quantities.

The negative sign in Eq.(4.166b) can be removed by imposing the condition that, for the states with positive k , the radial functions for the large and small components are

$$R_{nk}^{1*}(\rho) = -R_{nk}^1(\rho) , \quad (4.167a)$$

and

$$R_{nk}^{4*}(\rho) = -R_{nk}^4(\rho) , \quad (4.167b)$$

respectively.

All the relativistic states with $|k| = \frac{1}{2}$ exhibit a weak divergence of $R_{nk}^1(\rho)$ and $R_{nk}^4(\rho)$ at $\rho = 0$. As in the case of the relativistic three dimensional hydrogen atom (21), this is typical of the relativistic wave functions. In Figures 4.1 to 4.6 these radial functions multiplied by ρ are given in graphical form for $Z = 45$ together with the nonrelativistic $\rho R_{nl}(\rho)$. In order to do this, it is convenient to write the normalized relativistic radial functions in the series forms

$$\begin{cases} R_{nk}^1(\rho) \\ R_{nk}^4(\rho) \end{cases} = A_{nk} \rho^{\gamma_k - \frac{1}{2}} \exp(-\lambda_{nk}\rho) \sum_{J=0}^{\bar{n}} B_{nk}(J) \rho^J , \quad (4.168)$$

$$A_{nk} = \left\{ \frac{\Gamma(\bar{n} + 2\gamma_k + 1)}{4N_{nk}(N_{nk} - k) [\Gamma(2\gamma_k + 1)]^2 \bar{n}!} \right\}^{\frac{1}{2}} (2\lambda_{nk})^{\gamma_k + \frac{1}{2}} (1 \pm \epsilon_{nk})^{\frac{1}{2}} , \quad (4.169)$$

$$B_{nk} = \begin{cases} \pm(N_{nk} - k) - \bar{n} & ; \text{ for } J = 0 \\ \frac{(-2\lambda_{nk})^J}{\prod_{I=1}^J (2\gamma_k + I)} \binom{\bar{n}}{J} \left\{ \pm(N_{nk} - k) - (\bar{n} - J) \right\} & ; \text{ for } J \neq 0 \end{cases} \quad (4.170)$$

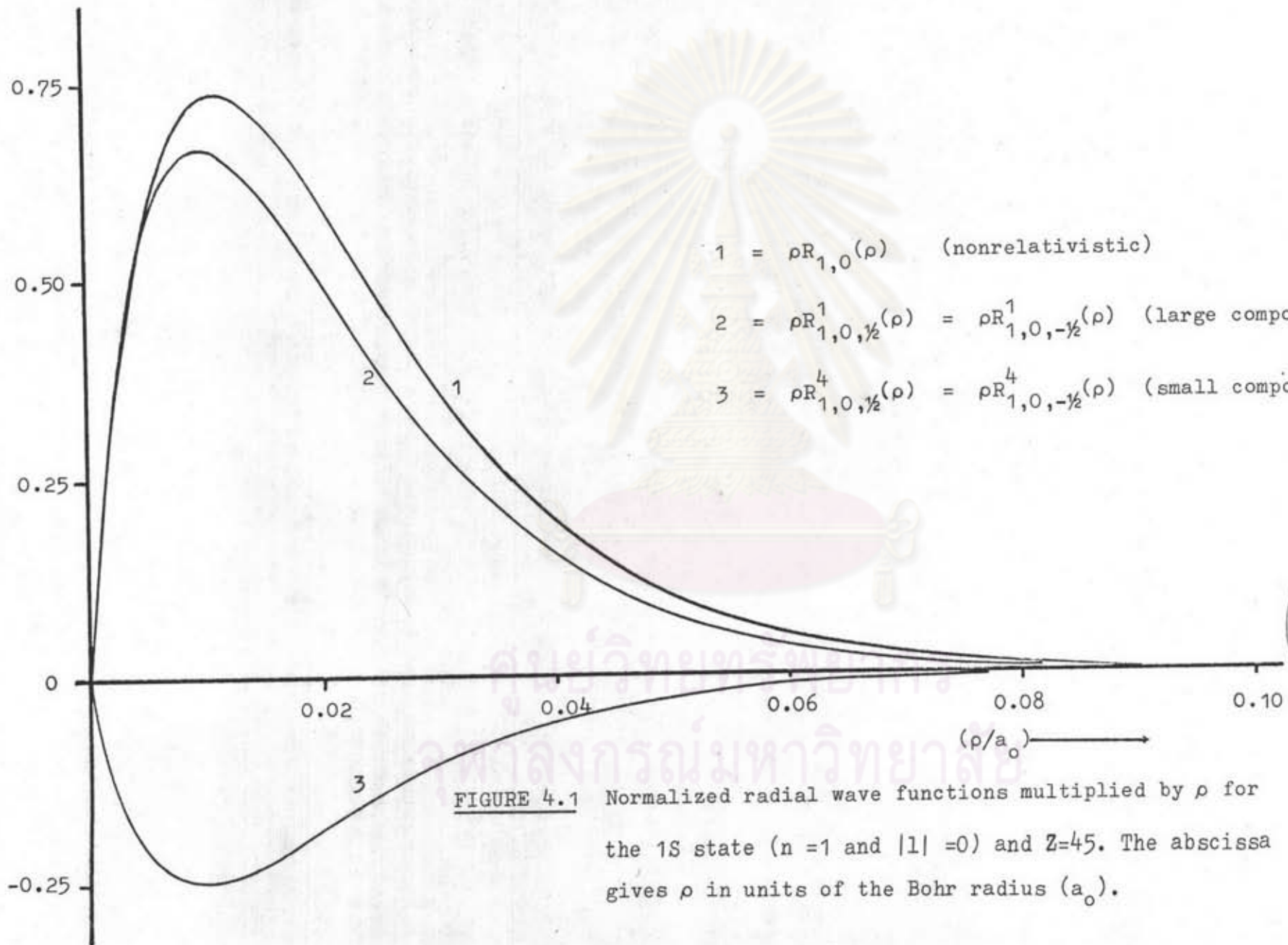


FIGURE 4.1 Normalized radial wave functions multiplied by ρ for the 1S state ($n=1$ and $|l|=0$) and $Z=45$. The abscissa gives ρ in units of the Bohr radius (a_0).



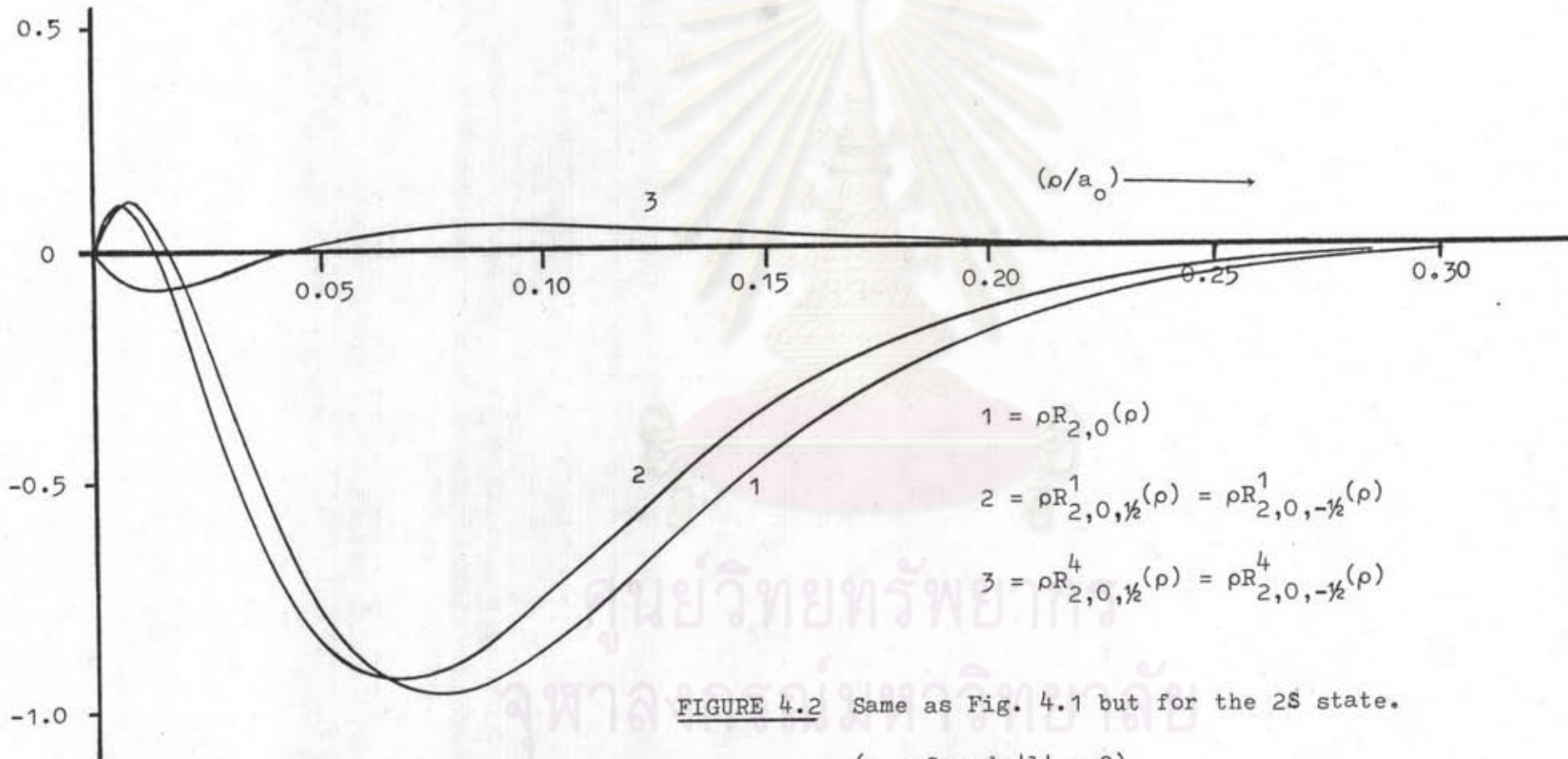


FIGURE 4.2 Same as Fig. 4.1 but for the 2S state.
 $(n = 2 \text{ and } |l| = 0)$

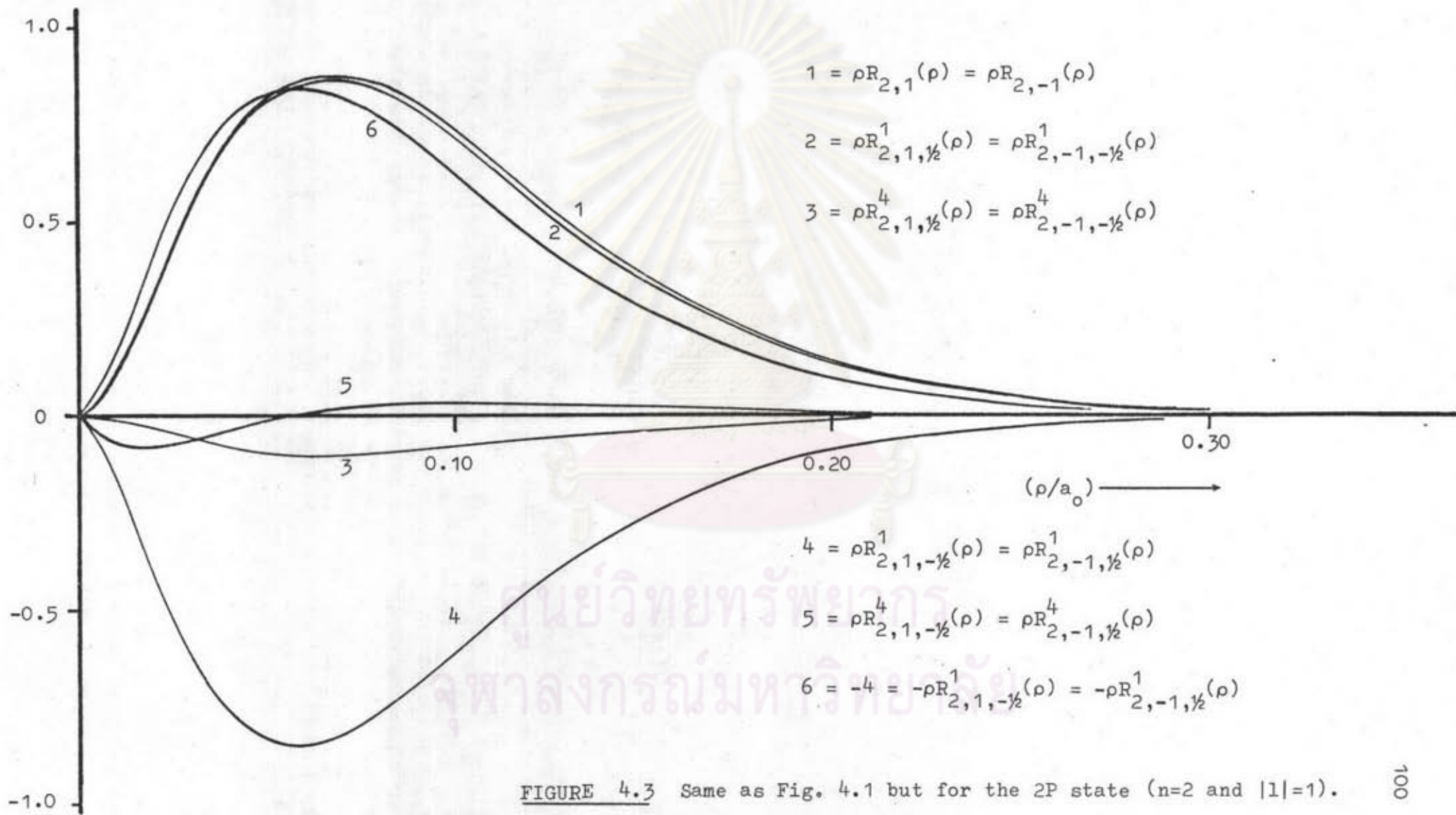


FIGURE 4.3 Same as Fig. 4.1 but for the 2P state ($n=2$ and $|l|=1$).

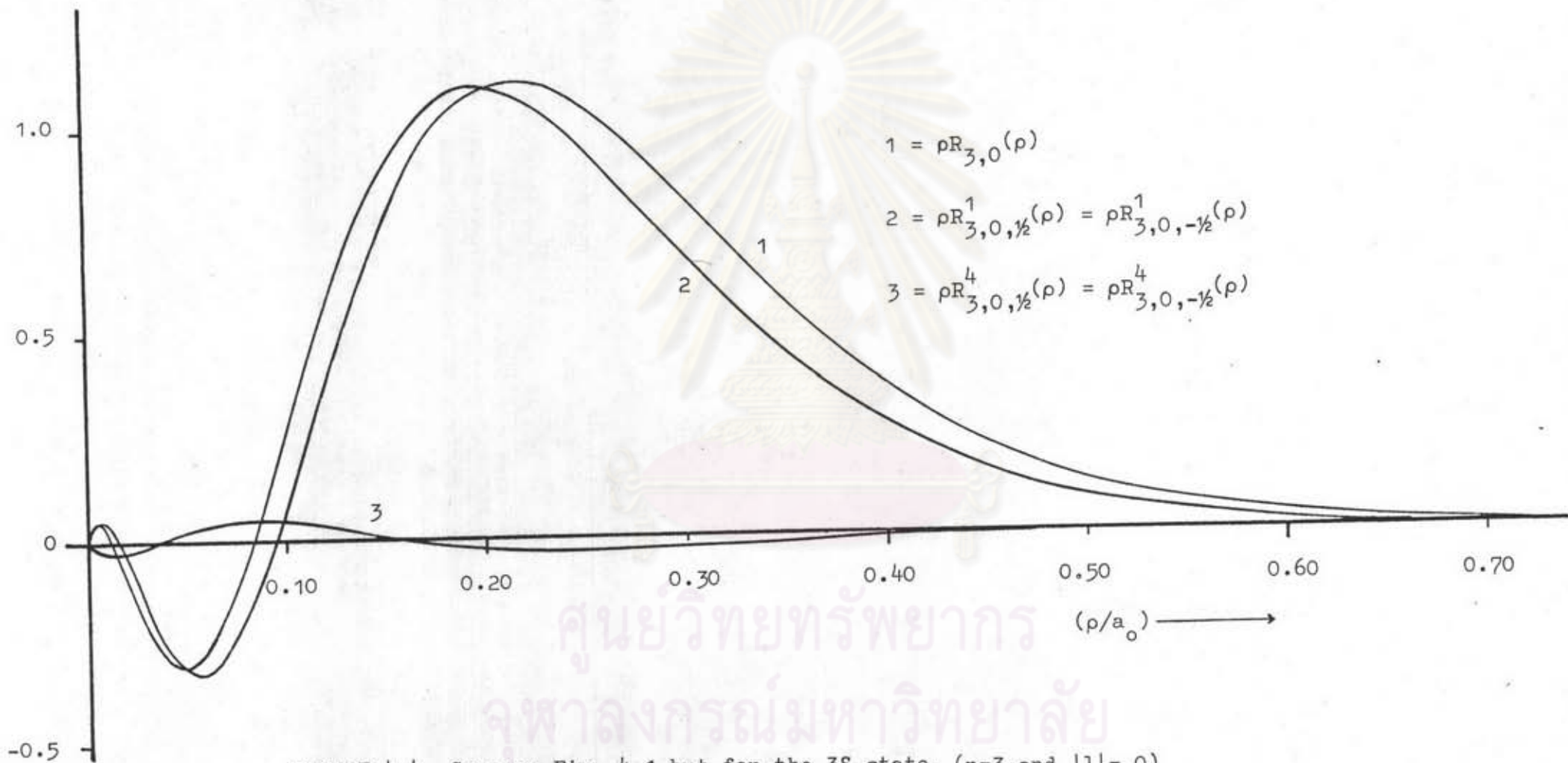


FIGURE 4.4 Same as Fig. 4.1 but for the 3S state. ($n=3$ and $|l|=0$)

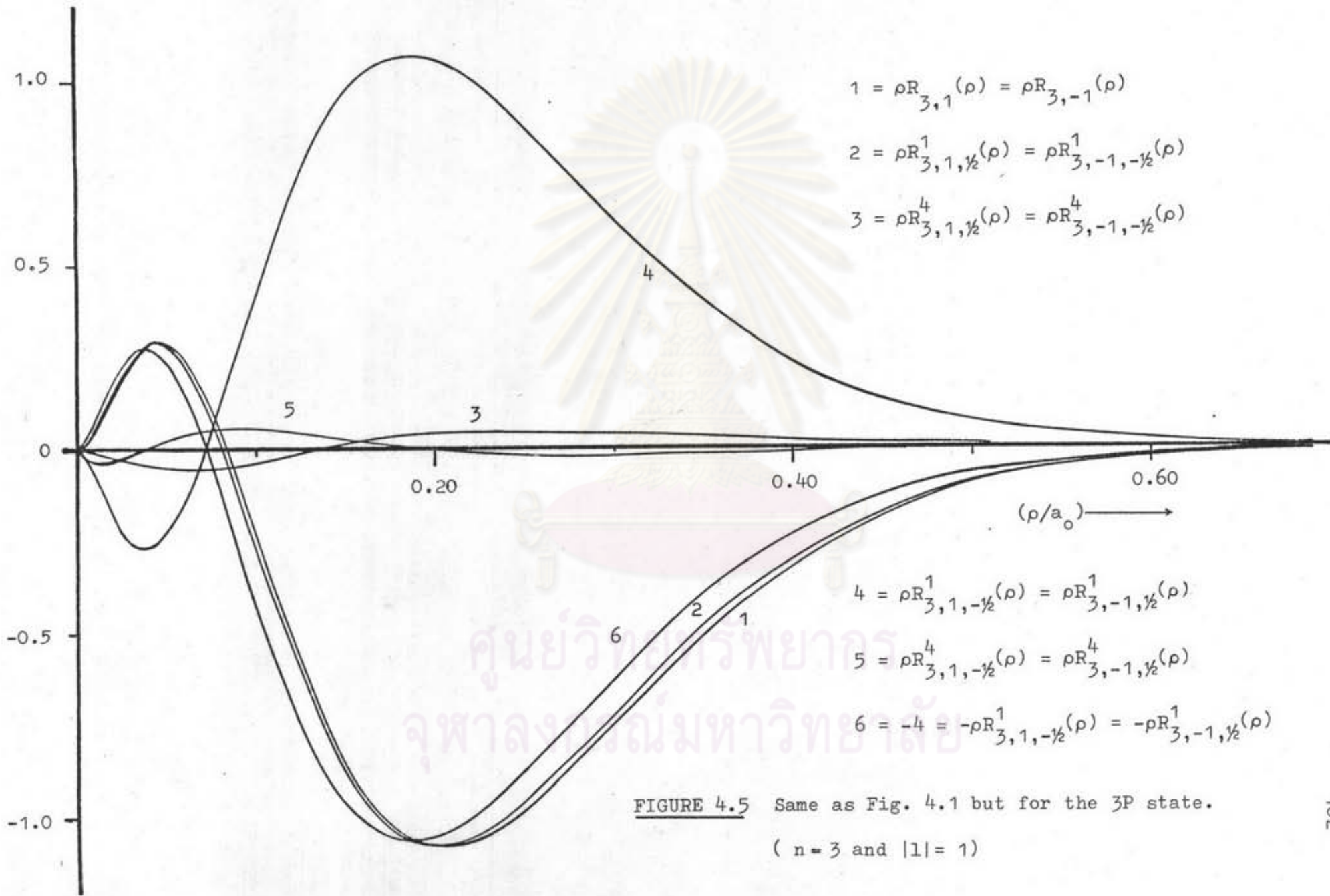


FIGURE 4.5 Same as Fig. 4.1 but for the 3P state.
(n = 3 and |l| = 1)

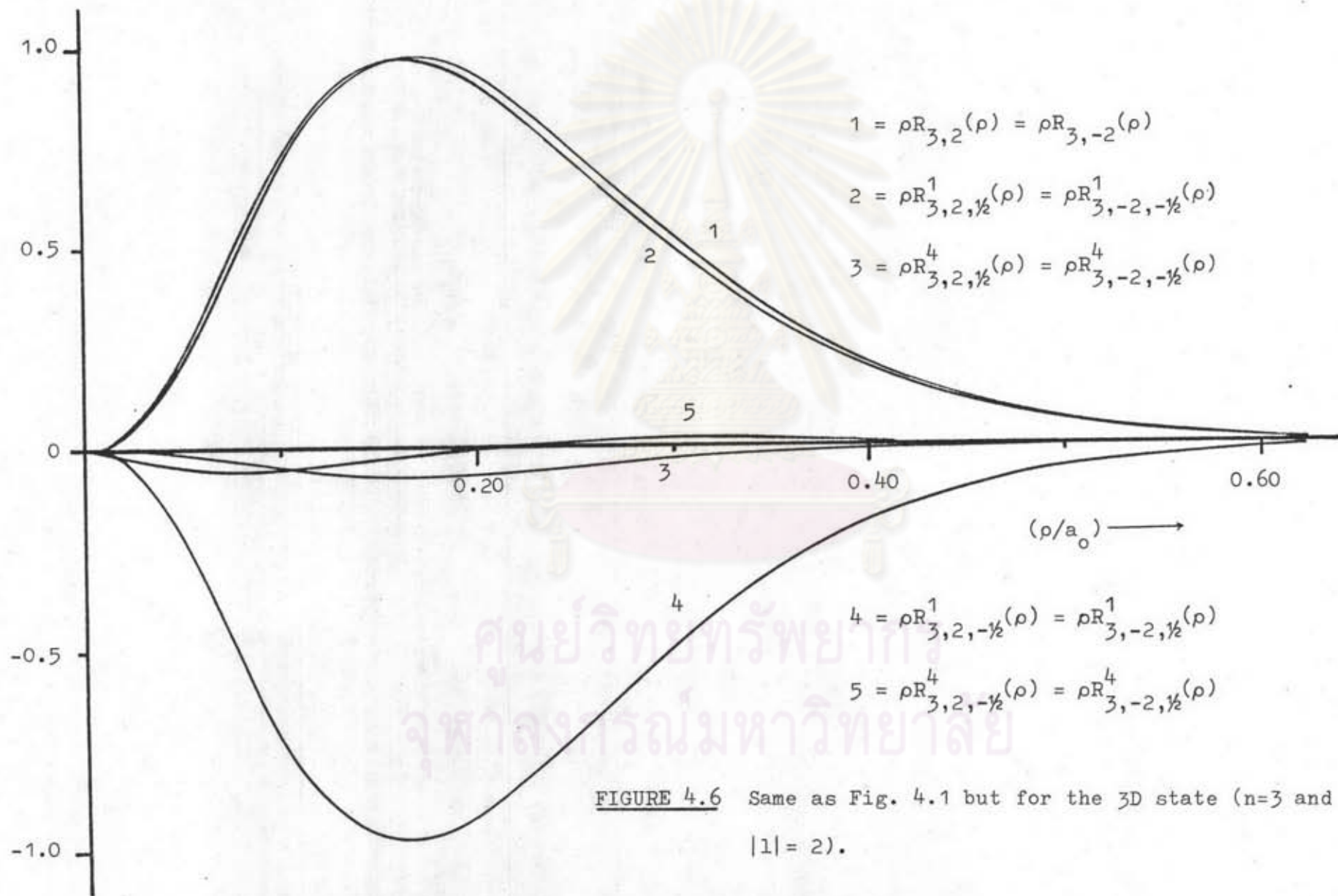


FIGURE 4.6 Same as Fig. 4.1 but for the 3D state (n=3 and |l|=2).

where the upper and lower signs stand for the large and small components, respectively ;

$$\prod_{I=1}^J (2\gamma_k + I) = (2\gamma_k+1)(2\gamma_k+2)\dots(2\gamma_k+J), \quad (4.171)$$

and

$$\binom{\bar{n}}{J} = \frac{\bar{n}!}{J!(\bar{n}-J)!} \quad (4.172)$$

The values of the gamma functions and of the square roots , with the accuracies of 10^{-10} and 10^{-17} , are obtained by means of the five-point Aitken's iteration method (48) and Newton's method (49), respectively. The program which we used to calculate A_{nk} and B_{nk} is given in Appendix C.

4.8 ENERGY SPECTRUM AND FINE STRUCTURE.

The energy eigenvalues for the relativistic two dimensional hydrogen atom, which have been derived in Section 4.5, are

$$\epsilon_{nk} = \frac{E_{nk}}{mc^2} = \left[1 + \left\{ \frac{Z\alpha}{(n-\frac{1}{2}) - |k| + (k^2 - (Z\alpha)^2)^{\frac{1}{2}}} \right\}^2 \right]^{-\frac{1}{2}}, \quad (4.103)$$

where the quantum numbers n and k are defined by Eqs.(4.39) and (4.102), namely

$$n = \bar{n} + |k| + \frac{1}{2} = 1, 2, 3, \dots, \quad (4.39)$$

$$k = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \pm\frac{7}{2}, \dots \quad (4.102)$$

Since the Sommerfeld fine structure constant, $\alpha = \frac{e^2}{\hbar c}$, is small, the parameter $(Z\alpha)$ in Eq.(4.103) will be small compared with unity, except for very large Z . It is therefore reasonable to expand Eq.(4.103) in ascending powers of $(Z\alpha)$:

$$\begin{aligned}
E_{nk} &= \frac{E_{nk}}{mc^2} = \left[1 + \left\{ \frac{Z\alpha}{(n-\frac{1}{2}) - |k| + (k^2 - (Z\alpha)^2)^{\frac{1}{2}}} \right\}^2 \right]^{-\frac{1}{2}} \\
&= \left[1 + \left\{ \frac{Z\alpha}{(n-\frac{1}{2}) - |k| + |k| \left\{ 1 - \frac{1}{2} \left(\frac{Z\alpha}{|k|} \right)^2 - \frac{1}{2 \cdot 4} \left(\frac{Z\alpha}{|k|} \right)^4 - \frac{1 \cdot 3}{2 \cdot 4 \cdot 6} \left(\frac{Z\alpha}{|k|} \right)^6 - \dots \right\}} \right\}^2 \right]^{-\frac{1}{2}} \\
&= \left[1 + \left(\frac{Z\alpha}{n-\frac{1}{2}} \right)^2 \left\{ \frac{1}{1 - \left(\frac{Z\alpha}{n-\frac{1}{2}} \right) \left\{ \frac{1}{2} \left(\frac{Z\alpha}{k} \right) + \frac{1}{2 \cdot 4} \left(\frac{Z\alpha}{k} \right)^3 + \dots \right\}} \right\}^2 \right]^{-\frac{1}{2}} \\
&= \left[1 + \left\{ M^2 (1-MN)^{-2} \right\} \right]^{-\frac{1}{2}} \\
&= 1 - \frac{1}{2} M^2 (1-MN)^{-2} + \frac{1 \cdot 3}{2 \cdot 4} \left[M^2 (1-MN)^{-2} \right]^2 \\
&\quad - \frac{1 \cdot 3 \cdot 5}{2 \cdot 4 \cdot 6} \left[M^2 (1-MN)^{-2} \right]^3 + \dots \\
&= 1 - \frac{1}{2} M^2 \left[1 + 2MN + 3(MN)^2 + 4(MN)^3 + \dots \right] \\
&\quad + \frac{1 \cdot 3}{2 \cdot 4} M^4 \left[1 + 4MN + 10(MN)^2 + 20(MN)^3 + \dots \right] \\
&\quad - \frac{1 \cdot 3 \cdot 5}{2 \cdot 4 \cdot 6} M^6 \left[1 + 6MN + 21(MN)^2 + 56(MN)^3 + \dots \right] + \dots \\
&= 1 - \frac{1}{2} \left(\frac{Z\alpha}{n-\frac{1}{2}} \right)^2 - \frac{1}{2} \left(\frac{Z\alpha}{n-\frac{1}{2}} \right)^4 \left[\left(\frac{n-\frac{1}{2}}{k} \right) - \frac{3}{4} \right] \\
&\quad - \frac{1}{8} \left(\frac{Z\alpha}{n-\frac{1}{2}} \right)^6 \left\{ \left(\frac{n-\frac{1}{2}}{k} \right)^3 + 3 \left(\frac{n-\frac{1}{2}}{k} \right)^2 - 6 \left(\frac{n-\frac{1}{2}}{k} \right) + \frac{5}{2} \right\} - \dots \quad (4.173)
\end{aligned}$$

or

$$\begin{aligned}
E_{nk} &= mc^2 - \frac{mc^2}{2} \left(\frac{Z\alpha}{n-\frac{1}{2}} \right)^2 - \frac{mc^2}{2} \left(\frac{Z\alpha}{n-\frac{1}{2}} \right)^4 \left[\left(\frac{n-\frac{1}{2}}{k} \right) - \frac{3}{4} \right] \\
&\quad - \frac{mc^2}{2} \left(\frac{Z\alpha}{n-\frac{1}{2}} \right)^6 \left\{ \left(\frac{n-\frac{1}{2}}{k} \right)^3 + 3 \left(\frac{n-\frac{1}{2}}{k} \right)^2 - 6 \left(\frac{n-\frac{1}{2}}{k} \right) + \frac{5}{2} \right\} \\
&\quad - \dots \quad (4.174)
\end{aligned}$$

where the abbreviated notations M and N are defined by

$$M = \left(\frac{Z\alpha}{n-\frac{1}{2}} \right) \quad \text{and} \quad N = \frac{1}{2} \left(\frac{Z\alpha}{k} \right) + \frac{1}{2 \cdot 4} \left(\frac{Z\alpha}{k} \right)^3 + \frac{1 \cdot 3}{2 \cdot 4 \cdot 6} \left(\frac{Z\alpha}{k} \right)^5 + \dots \quad (4.175)$$

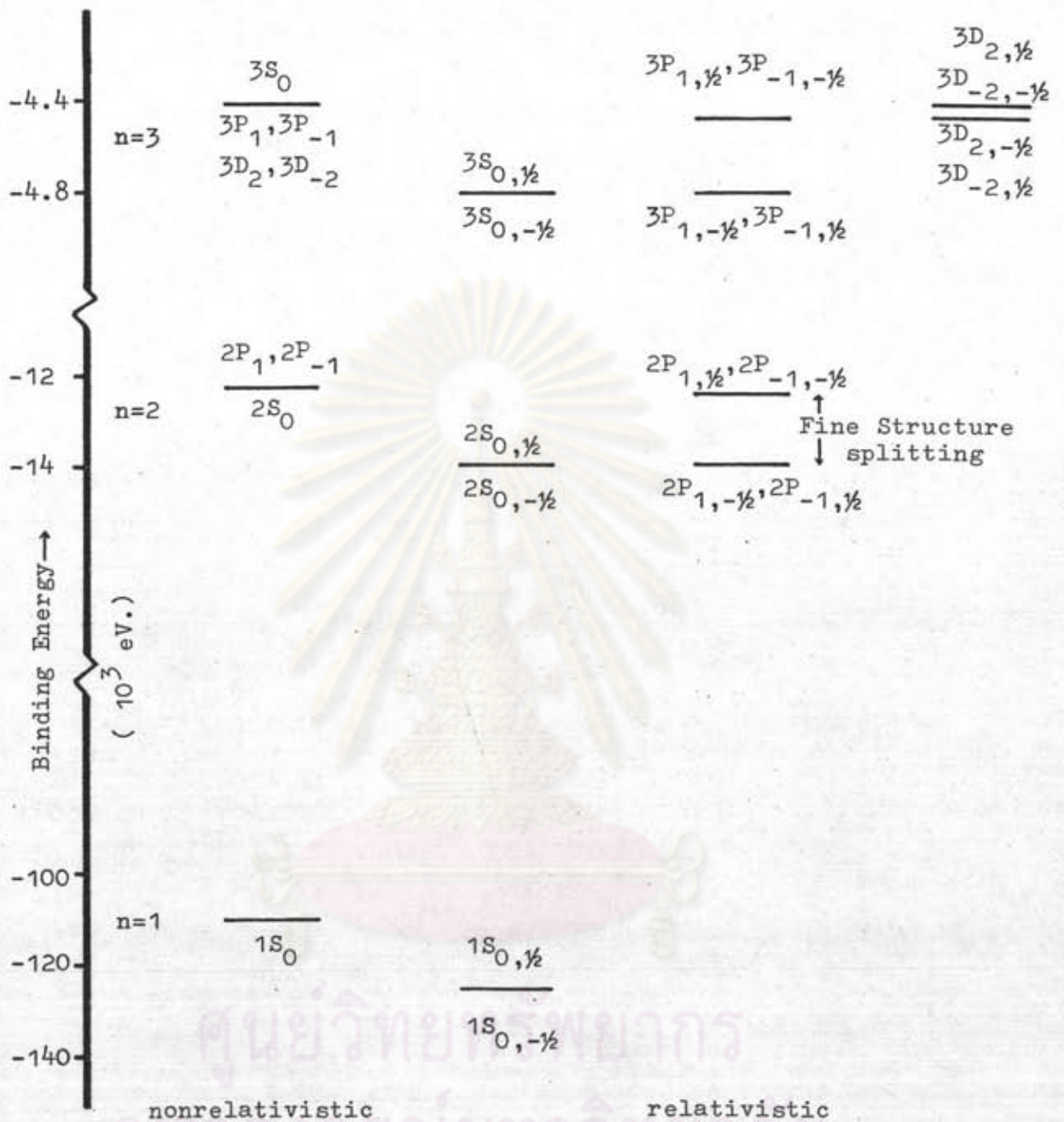


FIGURE 4.7 Energy level diagram of the relativistic two-dimensional hydrogen atom for $n = 1, 2,$ and 3 . The numerical values refer to the binding energy, $E_{nk} - mc^2$, and are calculated for the nonrelativistic and relativistic cases for $Z = 45$.

The first term on the right side of Eq.(4.174) is the rest energy of the electron. Comparing Eq.(4.174) with Eq.(3.31) we see that the second term gives the energy spectrum of the bound states of an electron in two-dimensional nonrelativistic hydrogen-like atom. The terms in $(Z\alpha)^4$ are exactly what is obtained in the nonrelativistic quantum theory (with spin) if a first order perturbation calculation is used to evaluate the contribution of the sum of the following three terms :

- (a) the additional energy due to the variation of mass with velocity

$$H_{\text{rel}} = -\frac{1}{2mc^2} (E - V)^2 ; \quad (4.176)$$

- (b) the spin-orbit interaction

$$H_{\text{sp}} = \frac{Ze^2\hbar}{4m^2c^2\rho^3} \sigma_z L_z ; \quad (4.177)$$

- (c) the two dimensional "Darwin" term, see Appendix B

$$H_{\text{Darwin}} = -\frac{Ze^2\hbar^2}{8m^2c^2\rho^3} . \quad (4.178)$$

The first term (a) contributes to E_{nk} the amount

$$\begin{aligned} E_{\text{rel}}^{(1)} &= \langle H_{\text{rel}} \rangle = -\frac{1}{2mc^2} \left\{ [E_n^{(0)}]^2 + 2E_n^{(0)}Ze^2 \langle \rho^{-1} \rangle \right. \\ &\quad \left. + Z^2e^4 \langle \rho^{-2} \rangle \right\} \\ &= -\frac{mc^2(Z\alpha)^4}{2(n - \frac{1}{2})^3} \left\{ \frac{1}{|1|} - \frac{1}{4(n - \frac{1}{2})} \right\} ; l \neq 0. \quad (4.179) \end{aligned}$$

The second term contributes

$$E_{nl, sp}^{(1)} = \begin{cases} \frac{mc^2(Z\alpha)^4}{2(n - \frac{1}{2})^3} \frac{1}{2|l|(|l| - \frac{1}{2})(|l| + \frac{1}{2})} ; j=l+\frac{1}{2} \text{ (spin-up), } l \neq 0, & (4.180a) \\ \frac{mc^2(Z\alpha)^4}{2(n - \frac{1}{2})^3} \frac{-1}{2|l|(|l| - \frac{1}{2})(|l| + \frac{1}{2})} ; j=l-\frac{1}{2} \text{ (spin-down), } l \neq 0, & (4.180b) \\ 0 ; l = 0 . & (4.180c) \end{cases}$$

Finally, the two dimensional Darwin term gives

$$\begin{aligned} E_{nl, Darwin}^{(1)} &= -\frac{Ze^2\hbar^2}{8m^2c^2} \langle \rho^{-3} \rangle \\ &= -\frac{Ze^2\hbar^2}{8m^2c^2} \left\{ \frac{m^3 Z^3 e^6}{\hbar^6 (n - \frac{1}{2})^3 |l|(|l| - \frac{1}{2})(|l| + \frac{1}{2})} \right\} \\ &= -\frac{mc^2(Z\alpha)^4}{2(n - \frac{1}{2})^3} \left\{ \frac{1}{4|l|(|l| - \frac{1}{2})(|l| + \frac{1}{2})} \right\} ; l \neq 0. \quad (4.181) \end{aligned}$$

Adding these we obtain

$$\begin{aligned} E_{rel}^{(1)} + E_{nl, sp}^{(1)} + E_{nl, Darwin}^{(1)} &= -\frac{mc^2(Z\alpha)^4}{2(n - \frac{1}{2})^3} \left\{ \frac{1}{|l|} \mp \frac{1}{2|l|(|l| - \frac{1}{2})(|l| + \frac{1}{2})} \right. \\ &\quad \left. + \frac{1}{4|l|(|l| - \frac{1}{2})(|l| + \frac{1}{2})} - \frac{3}{4(n - \frac{1}{2})} \right\}; l \neq 0 \\ &= -\frac{mc^2(Z\alpha)^4}{2(n - \frac{1}{2})^3} \left\{ \frac{1}{|l|} + \frac{1 \mp 2l}{4|l|(|l| - \frac{1}{2})(|l| + \frac{1}{2})} \right. \\ &\quad \left. - \frac{3}{4(n - \frac{1}{2})} \right\}; l \neq 0, \quad (4.182) \end{aligned}$$

where the upper and lower signs stand for the spin-up and spin-down states, respectively. For positive l , $l > 0$, the above equations reduce to

$$E_{\text{rel}}^{(1)} + E_{\text{sp}}^{(1)} + E_{\text{Darwin}}^{(1)} = -\frac{mc^2(Z\alpha)^4}{2(n-\frac{1}{2})^3} \left\{ \frac{1}{(|l|\pm\frac{1}{2})} - \frac{3}{4(n-\frac{1}{2})} \right\}, \quad (4.183)$$

and for negative l , $l < 0$,

$$E_{\text{rel}}^{(1)} + E_{\text{sp}}^{(1)} + E_{\text{Darwin}}^{(1)} = -\frac{mc^2(Z\alpha)^4}{2(n-\frac{1}{2})^3} \left\{ \frac{1}{(|l|\mp\frac{1}{2})} - \frac{3}{4(n-\frac{1}{2})} \right\}. \quad (4.184)$$

In terms of the quantum number k ,

$$k = \begin{cases} -j & \text{for } j = l + \frac{1}{2} \text{ (spin-up)} \\ j & \text{for } j = l - \frac{1}{2} \text{ (spin-down)} \end{cases}, \quad (4.185)$$

both Eqs.(4.183) and (4.184) can be written as

$$E_{\text{rel}}^{(1)} + E_{\text{sp}}^{(1)} + E_{\text{Darwin}}^{(1)} = -\frac{mc^2(Z\alpha)^4}{2(n-\frac{1}{2})^4} \left\{ \frac{(n-\frac{1}{2})}{|k|} - \frac{3}{4} \right\}; \quad l \neq 0, \quad (4.186)$$

which confirm the validity of the statement made above provided that Eq.(4.186) is extended to include the cases in which $l = 0$.

Fine Structure : Since, as can be seen from Table 4.1, for a given value of the 'principal' quantum number n , there are n possible values of $|k|$ and therefore n different values of the energy eigenvalues E_{nk} , the complete degeneracy of a given n in the non-relativistic case is lifted by relativistic effects leading to the so-called 'fine structure splitting' of the energy levels. However, there still remains a degeneracy of the states with same n and $|k|$ but differ in either k , j , or l . For example, the $2S_{0,\frac{1}{2}}$, $2S_{0,-\frac{1}{2}}$, $2P_{1,-\frac{1}{2}}$ and $2P_{-1,\frac{1}{2}}$ levels are degenerate. The energies of the low-lying states have been represented on Figure 4.7 for $Z = 45$.

According to Eq.(4.174), the difference in energy between the states of the same n but of different $|k|$, $|k|$ and $|k|-1$, is

$$\begin{aligned} \Delta E_{n, |k|} &= E_{n, |k|} - E_{n, |k|-1} \\ &= \frac{mc^2(Z\alpha)^4}{2(n-\frac{1}{2})^4} \left\{ \frac{(n-\frac{1}{2})}{|k|^2 - |k|} + \frac{mc^2(Z\alpha)^6}{8(n-\frac{1}{2})^6} \left[(n-\frac{1}{2})^3 \left\{ \frac{|k|^3 - (|k|-1)^3}{|k|^3 (|k|-1)^3} \right\} \right. \right. \\ &\quad \left. \left. + 3(n-\frac{1}{2})^2 \left\{ \frac{|k|^2 - (|k|-1)^2}{|k|^2 (|k|-1)^2} - \frac{6(n-\frac{1}{2})}{(|k|^2 - |k|)} \right\} \right] \right\}. \quad (4.187) \end{aligned}$$

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