CHAPTER III

NONRELATIVISTIC TWO DIMENSIONAL HYDROGEN ATOM

In this chapter we will study the problem of the two dimensional hydrogen atom by means of the nonrelativistic quantum mechanics. First, in Section 3.1, we study the Schroedinger nonrelativistic quantum mechanical treatment of the problem in position space which has been discussed by Zaslow and Zandler (9), Huang and Kozycki (10), and by Hassoun (11). Then, the extension to include the spin and relativistic effects will be made in Sections 3.2 and 3.3, respectively.

3.1 THE SCHROEDINGER WAVE MECHANICAL TREATMENT OF TWO DIMENSIONAL HYDROGEN ATOM.

The time independent Schroedinger equation for the two dimensional hydrogen atom, the system in which a single electron moves in a plane around the nucleus under the influence of the attractive Coulomb potential $V(\rho) = - Ze^2/\rho$, is

$$HU(\rho,\phi) = (- \frac{\hbar^2}{2m}\nabla^2 + V(\rho))U(\rho,\phi) = EU(\rho,\phi) \qquad (3.1)$$

where

$$\nabla^2 = \frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} \qquad (3.2)$$

in the two dimensional polar coordinates (ρ, ϕ), m is the mass of the electron, E is the energy eigenvalue, and $U(\rho, \phi)$ is the wave function associated with E. In order to solve Eq.(3.1) we first separate the radial and the angular parts by substituting

$$U(\rho, \phi) = R(\rho)\phi(\phi) \qquad (3.3)$$

into Eq.(3.1) and dividing throughout by $U(\rho,\phi)$:

$$\left[\frac{\rho^2}{R(\rho)}\frac{d^2}{d\rho^2} + \frac{\rho}{R(\rho)}\frac{d}{d\rho} + \frac{2m\rho^2}{\hbar^2}(E + \frac{Ze^2}{\rho})\right] R(\rho) = -\frac{1}{\phi(\phi)}\frac{d^2}{d\phi^2} \phi(\phi) \qquad (3.4)$$

Since the left side of Eq.(3.4) depends only on ρ where as the right side depends only on ϕ, both sides must be equal to a constant that we call 1^2. Thus Eq.(3.4) gives us a radial equation

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} + \frac{2m}{\hbar^2}(E + \frac{Ze^2}{\rho}) - \frac{1^2}{\rho^2}\right] R(\rho) = 0 \qquad (3.5)$$

and an angular equation

$$\frac{d^2}{d\phi^2} \phi(\phi) + 1^2 \phi(\phi) = 0 . \qquad (3.6)$$

The angular equation (3.6) can be solved at once: its general solution may be written

$$\phi(\phi) = \begin{cases} Ae^{il\phi} + Be^{-il\phi} & , 1^2 \neq 0 \\ A + B\phi & , 1^2 = 0 . \end{cases} \qquad (3.7)$$

The requirement that $\phi(\phi)$ and $\phi'(\phi)$ be continuous through out the domain $\phi = 0$ to 2π demands that 1 must be a positive or negative integer or zero. We thus replace Eq,(3.7) by

$$\phi_1(\phi) = (2\pi)^{-\frac{1}{2}} \exp(il\phi) , \qquad (3.8)$$

where the multiplying constant is chosen equal to $(1/2\pi)^{\frac{1}{2}}$ in order that $\phi(\phi)$ be normalized to unity over the range of ϕ :

$$\int_0^{2\pi} \phi_1^*(\phi)\phi_1(\phi)d\phi = 1 \qquad (3.9)$$

The subscript 1 is added to denote the dependence of $\phi(\phi)$ on 1.

The radial equation that corresponds to the quantum number l is

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} + \frac{2m}{\hbar^2}\left(E + \frac{Ze^2}{\rho}\right) - \frac{l^2}{\rho^2} \right] R(\rho) = 0 \tag{3.10}$$

where $l = 0, \pm 1, \pm 2, \ldots$. It is convenient in dealing with an equation of this type to rewrite it in dimensionless form. For this purpose we introduce (a) the atomic unit of length, the Bohr radius :

$$a_o = \hbar^2/me^2 \quad, \tag{3.11}$$

(b) the atomic unit of energy :

$$E_{at} = e^2/a_o = me^4/\hbar^2 \tag{3.12}$$

and (c) the dimensionless quantities $\bar{\rho}$ and ϵ :

$$\bar{\rho} = \rho/a_o \quad, \quad \epsilon = E/E_{at} \tag{3.13}$$

Equation (3.10) then becomes

$$\left[\frac{d^2}{d\bar{\rho}^2} + \frac{1}{\bar{\rho}}\frac{d}{d\bar{\rho}} + 2\epsilon + \frac{2Z}{\bar{\rho}} - \frac{l^2}{\bar{\rho}^2} \right] R(\bar{\rho}) = 0 \tag{3.14}$$

For the bound state , $E < 0$, it is convenient to introduce a positive quantity α^2 by the equation

$$\alpha^2 = -2\epsilon > 0 \tag{3.15}$$

Thus, the dimensionless form of the radial equation for the bound state is

$$\left[\frac{d^2}{d\bar{\rho}^2} + \frac{1}{\bar{\rho}}\frac{d}{d\bar{\rho}} - \alpha^2 + \frac{2Z}{\bar{\rho}} - \frac{l^2}{\bar{\rho}^2} \right] R(\bar{\rho}) = 0 \tag{3.16}$$

3.1.1 <u>Asymptotic Behavior</u> : The solution of Eq.(3.16) is facilitated by first examining the dominant behavior of $R(\bar{\rho})$ in the asymptotic regions $\bar{\rho} \to 0$ and $\bar{\rho} \to \infty$. For sufficiently small $\bar{\rho}$ we can omit the third and the forth terms , Eq.(3.16) is then reduced to

$$\left[\frac{d^2}{d\bar{\rho}^2} + \frac{1}{\bar{\rho}} \frac{d}{d\bar{\rho}} - \frac{1^2}{\bar{\rho}^2} \right] R(\bar{\rho}) = 0 \qquad (3.17)$$

Assuming

$$\frac{R(\bar{\rho})}{\bar{\rho} \to 0} = \bar{\rho}^{\gamma} \qquad (3.18)$$

we get the condition

$$\gamma^2 = 1^2 \qquad (3.19)$$

Since the wave function must be finite at the origin, the negative roots of γ must be excluded. We thus get

$$\gamma = |1| \qquad (3.20)$$

and

$$\frac{R(\bar{\rho})}{\bar{\rho} \to 0} = \bar{\rho}^{|1|} \qquad (3.21)$$

For sufficiently large $\bar{\rho}$ we can neglect in Eq. (3.16) the second, the forth, and the last terms :

$$\left[\frac{d^2}{d\bar{\rho}^2} - \alpha^2 \right] R(\bar{\rho}) = 0 \qquad (3.22)$$

Thus, the asymptotic solution of Eq. (3.16) for large $\bar{\rho}$ must be of the form

$$\frac{R(\bar{o})}{\bar{\rho} \to \infty} = A \exp(-\alpha\bar{\rho}) + B \exp(\alpha\bar{\rho}) \qquad (3.23)$$

As the wave function must remain finite as $\bar{\rho}$ tends to infinity we must have B = 0.

3.1.2 General Solution of the Radial Equation : From the asymptotic bahavior of the radial function we can write the solution of Eq. (3.16) for all values of $\bar{\rho}$ in the form

$$R(\bar{\rho}) = \exp(-\alpha\bar{\rho}) \, \bar{\rho}^{\gamma} \, F(\bar{\rho}) \qquad (3.24)$$

where $F(\bar{\rho})$ is a power series

$$F(\bar{\rho}) = \sum_{s=0}^{\infty} \beta_s \bar{\rho}^s \qquad . \tag{3.25}$$

Substituting Eq. (3.24) into Eq. (3.16), we obtain

$$-\sum_{s=0}^{\infty} (\alpha(2\gamma+1)+2\alpha s-2Z)\beta_s \bar{\rho}^{+s-1} + \sum_{s=0}^{\infty} s(2\gamma+s)\beta_s \bar{\rho}^{+s-2} = 0 \quad . \tag{3.26}$$

The recusion relation between the coefficients of successive terms of the series (3.25) can be obtained by equating to zero the coefficient of the term of power $(\gamma+s-2)$. The result is

$$\frac{\beta_s}{\beta_{s-1}} = \frac{\alpha(2\gamma+1) + 2\alpha(s-1)-2Z}{s(2\gamma+s)} \quad . \tag{3.27}$$

3.1.3 <u>Quantum Condition and Energy Levels</u> : It follows from Eq. (3.27) that the coefficients of the terms of very high power, $s\rightarrow\infty$, satisfy the abbreviated recursion.

$$\frac{\beta_s}{\beta_{s-1}} \longrightarrow \frac{2\alpha}{s} \quad , \tag{3.28}$$

which is the same as that of the series for $\exp(2\alpha\bar{\rho})$. This ratio permits the conclusion that for large $\bar{\rho}$ the function $F(\bar{\rho})$ behaves asymptotically as $\exp(2\alpha\bar{\rho})$. Eq. (3.24) shows that this behavior for $F(\bar{\rho})$ violates the boundary condition on $R(\bar{\rho})$ for large $\bar{\rho}$. Hence, the series (3.25) must terminate. If the highest power of $\bar{\rho}$ is $\bar{n}$, $\bar{n} \geqslant 0$, i.e., $F(\bar{\rho})$ is the polynomial of degree $\bar{n}$, then $\beta_{\bar{n}} \neq 0$ but $\beta_{\bar{n}+1} = 0$. With $s = \bar{n}+1$, Eq. (3.27) leads to the "quantum condition"

$$\alpha(2\gamma+1) + 2\alpha\bar{n} - 2Z = 0 \quad , \tag{3.29a}$$

or

$$Z = \alpha(\bar{n} + \gamma + \tfrac{1}{2}) \tag{3.29b}$$

Since, from Eqs. (3.15), (3.13) and (3.12),

$$\alpha^2 = -\frac{2E\hbar^2}{me^4} \tag{3.30}$$

and $\gamma = |1|$,we can solve for the energy eigenvalues E ;

$$E_n = - \frac{mZ^2 e^4}{2\hbar^2(\bar{n}+|1|+\frac{1}{2})^2} = - \frac{mZ^2 e^4}{2\hbar^2(n-\frac{1}{2})^2} \tag{3.31}$$

where n is the new quantum number defined by the equation

$$n = \bar{n} + |1| + 1 \tag{3.32}$$

Eq. (3.31) indicates that, using the three dimensional hydrogen atom as a reference, the energy levels are lower in the planar case. For the ground state, the energy of the planar atom is four times that of the three dimensional atom. The low-lying energy levels of the two dimensional hydrogen atom (Z = 1)are shown in Figure 3.1.

Substituting Eq. (3.29b) into Eq.(3.27), we obtain

$$\beta_s = \frac{2\alpha(-n+|1|+s)}{s(2\gamma+s)} \beta_{s-1} \tag{3.33}$$

This implies that

$$F(\bar{\rho}) = \beta_0 + \beta_1\bar{\rho} + \beta_2\bar{\rho}^2 + \beta_3\bar{\rho}^3 + \ldots$$

$$= \beta_0 + \frac{2\alpha(-n+|1|+1)}{(2|1|+1)}\beta_0\bar{\rho} + \frac{(2\alpha)^2(-n+|1|+1)(-n+|1|+2)}{2!(2|1|+1)(2|1|+2)}\beta_0\bar{\rho}^2$$

$$+ \frac{(2\alpha)^3(-n+|1|+1)(-n+|1|+2)(-n+|1|+3)}{3!(2|1|+1)(2|1|+2)(2|1|+3)} \beta_0\bar{\rho}^3 + \ldots$$

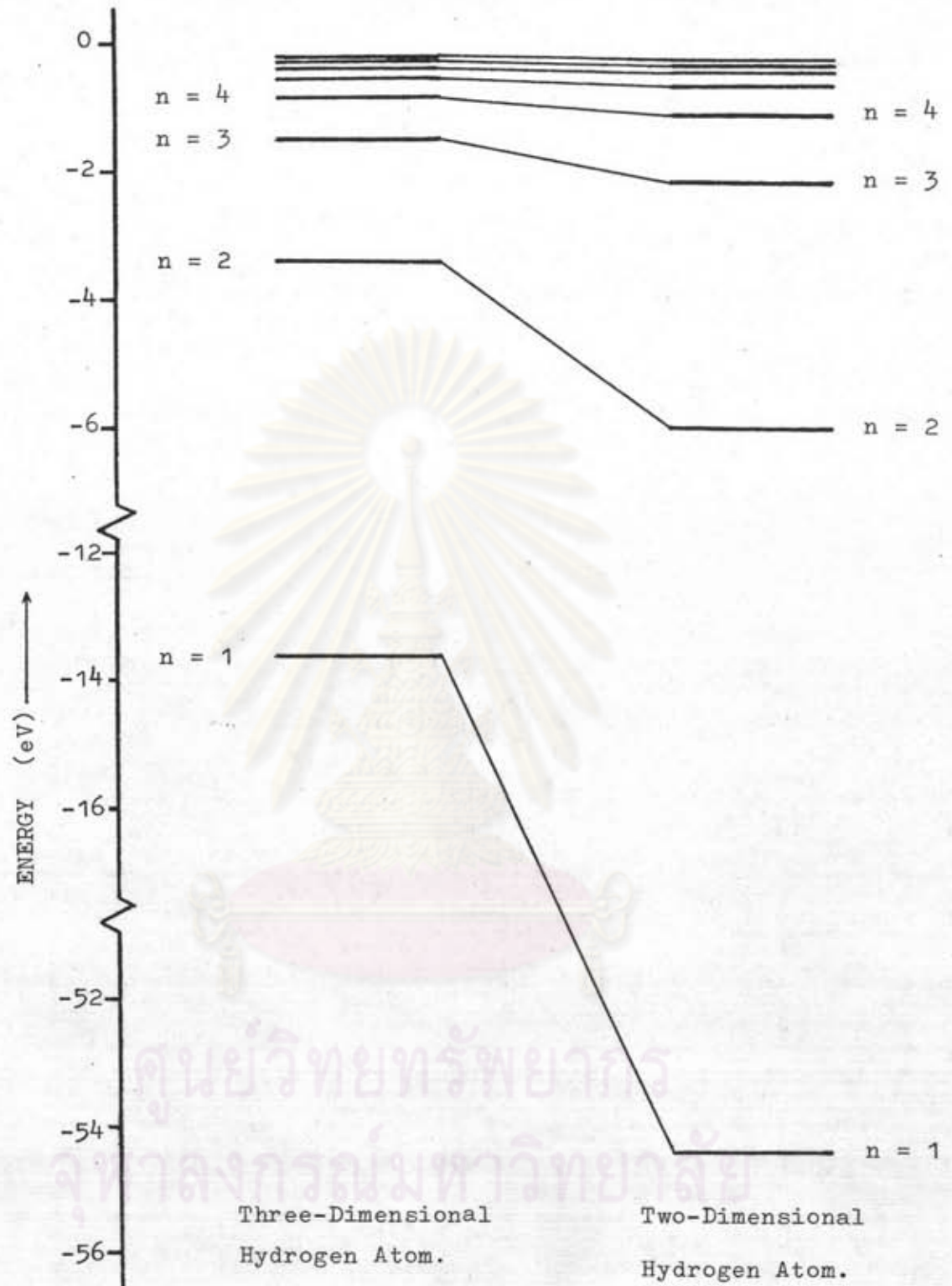$$= \beta_0 \, {}_1F_1(-n+|1|+1; 2|1|+1; 2\alpha\bar{\rho}) \tag{3.34}$$

where ${}_1F_1(a; c; z)$ is the confluent hypergeometric function

$$ {}_1F_1(a; c; z) = 1 + \frac{a}{c}z + \frac{a(a+1)}{c(c+1)}\frac{z^2}{2!} + \frac{a(a+1)(a+2)}{c(c+1)(c+2)}\frac{z^3}{3!} +\ldots \tag{3.35}$$

The radial part of the wave function $R(\bar{\rho})$ is thus

$$R_{n1}(\bar{\rho}) = \beta_0\exp(-\alpha\bar{\rho})\,\bar{\rho}^{|1|}\,{}_1F_1(-n+|1|+1; 2|1|+1; 2\alpha\bar{\rho}) \tag{3.36}$$

FIGURE 3.1 Low-lying energy levels of the nonrelativistic

two-dimensional hydrogen atom (Z = 1). The left

portion shows the energy levels of the

nonrelativistic three-dimensional hydrogen atom.

where β_o is a constant factor to be determined from the normalization condition. The subscripts n and l are added to indicate the dependence of $R(\bar{\rho})$ on the quantum numbers n and l.

3.1.4 <u>Normalized Wave Functions</u> : Since the motion of the electron around the nucleus is constrainted to be planar, the normalization condition is, in the plane polar coordinates (ρ, ϕ),

$$\int_{\text{over the plane}} U_{nl}^{+}(\rho,\phi)U_{nl}(\rho,\phi)\rho d\rho d\phi = 1 . \qquad (3.37)$$

The angular part of the wave function is already chosen to satisfy the angular normalization condition (3.9), Eq.(3.37) then requires that the radial normalization condition

$$\int_0^\infty R_{nl}^{+}(\rho)R_{nl}(\rho)\rho d\rho = 1 \qquad (3.38)$$

be satisfied. Writing Eq.(3.38) in terms of the dimensionless variable $\bar{\rho}$ yields

$$\int_0^\infty R_{nl}^{+}(\bar{\rho})R_{nl}(\bar{\rho})\bar{\rho}d\bar{\rho} = 1/a_o^2 . \qquad (3.39)$$

Using Eq.(3.36), we obtain

$$\frac{\beta_o^2}{(2\alpha)^{2|l|+2}} \int_0^\infty e^{-z} z^{2|l|+1} \left[{}_1F_1(-n+|l|+1; 2|l|+1; z) \right]^2 dz = \frac{1}{a_o^2} \qquad (3.40)$$

where $z = 2\alpha\bar{\rho}$. Since, from Appendix A,

$$\int_0^\infty e^{-z} z^{2|l|+1} \left[{}_1F_1(-n+|l|+1; 2|l|+1; z) \right]^2 dz$$

$$= \frac{[\Gamma(2|l|+1)]^2 \Gamma(n-|l|)}{\Gamma(n+|l|)}(2n-1) \qquad (3.41)$$

Eq.(3.40) then gives

$$\beta_o = \left[\frac{\Gamma(n+|l|)}{[\Gamma(2|l|+1)]^2 \Gamma(n-|l|)(2n-1)} \right]^{1/2} \left(\frac{2\alpha}{a_o}\right)(2\alpha)^{|l|} . \qquad (3.42)$$

Thus the normalized wave functions for the two dimensional hydrogen atom are

$$U_{nl}(\rho,\phi) = R_{nl}(\rho)\,\phi_l(\phi) \tag{3.43a}$$

$$R_{nl}(\rho) = \beta\left[\frac{\Gamma(n+|l|)}{[\Gamma(2|l|+1)]^2\,\Gamma(n-|l|)(2n-1)}\right]^{\frac{1}{2}} \exp(-\tfrac{1}{2}\beta\rho)\,(\beta\rho)^{|l|}$$

$$X\quad {}_1F_1(-n+|l|+1;\,2|l|+1;\,\beta\rho) \tag{3.43b}$$

$$\phi_l(\phi) = (2\pi)^{-\frac{1}{2}}\exp(il\phi) \tag{3.43c}$$

where β is defined by the relation

$$\beta = \frac{2\alpha}{a_o} = \frac{2mZe^2}{\hbar^2(n-\frac{1}{2})} = \frac{4Z}{a_o(2n-1)} \quad . \tag{3.44}$$

As can be seen from Eq.(3.32), for a given value of the quantum number n, the possible values of l are $0,\pm1,\pm2,\pm3,\ldots,\pm(n-1)$. The corresponding energy eigenvalues are

$$E_n = -\frac{mZ^2e^4}{2\hbar^2(n-\frac{1}{2})^2} \tag{3.45}$$

The radial part of the wave functions can also be expressed in terms of the generalized Laguerre polynomials ;

$$R_{nl}(\rho) = \beta\left[\frac{\Gamma(n-|l|)}{\Gamma(n+|l|)(2n-1)}\right]^{\frac{1}{2}} \exp(-\tfrac{1}{2}\beta\rho)\,(\beta\rho)^{|l|}\,\mathcal{L}_{n-|l|-1}^{(2|l|)}(\beta\rho), \tag{3.46}$$

where the generalized Laguerre polynomials $\mathcal{L}_n^{(c)}(z)$ is defined in terms of the confluent hypergeometric functions as [38]

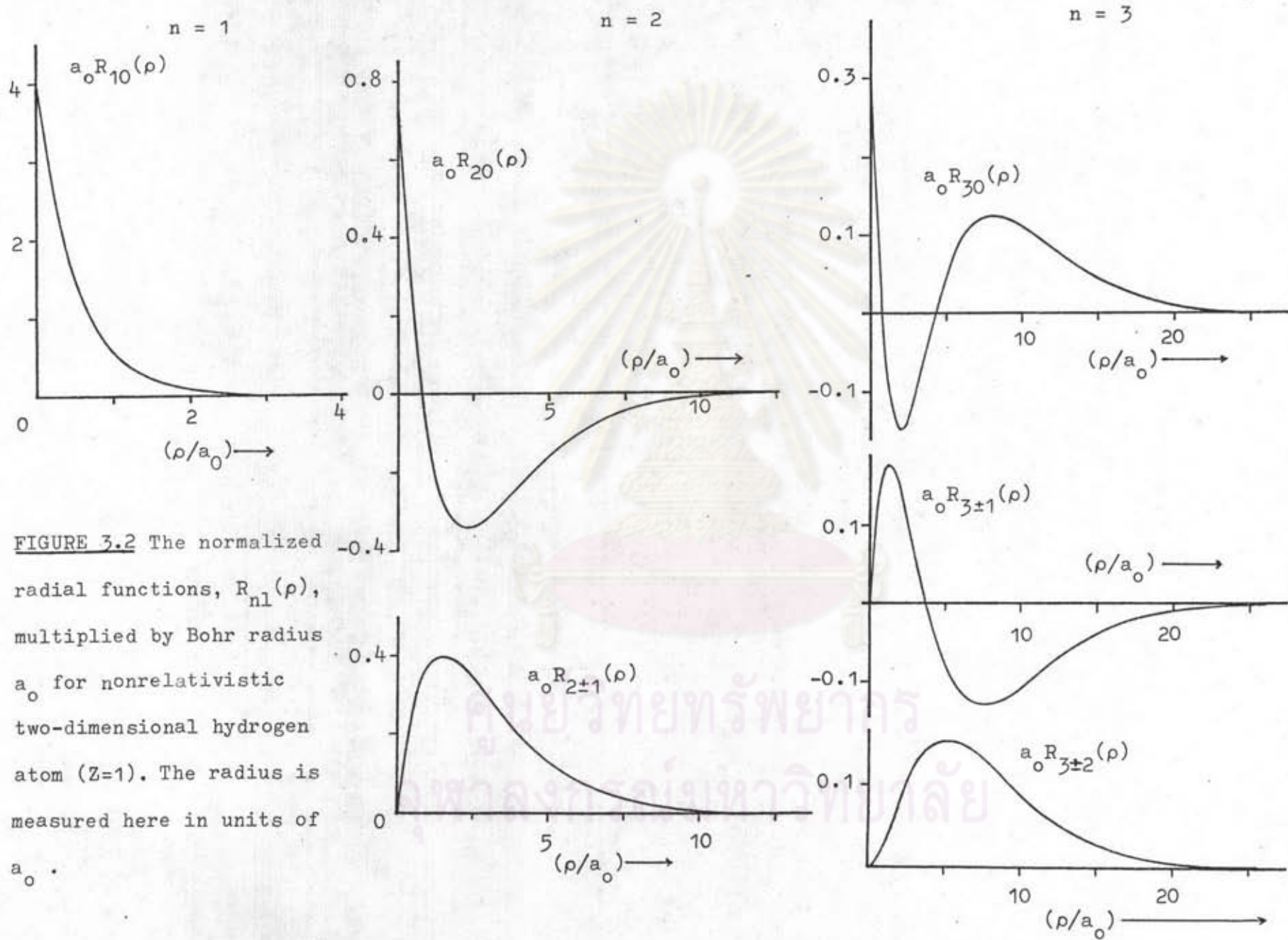$$\mathcal{L}_n^{(c)}(z) = \frac{\Gamma(c+n+1)}{n!\,\Gamma(c+1)}\,{}_1F_1(-n;\,c+1;\,z) \quad , \tag{3.47}$$

n is any non-negative integer and c may be any complex number.

Table 3.1 is a listing of the normalized radial functions $R_{nl}(o)$ for n=1, 2, 3, 4. In Figure 3.2, these radial functions are given in graphical form for Z=1.

<u>TABLE 3.1</u> The normalized radial functions for the states with

n = 1, 2, 3, 4.

$$R_{nl}(\rho) = \frac{\beta}{\Gamma(2|l|+1)} \left[\frac{\Gamma(n+|l|)}{\Gamma(n-|l|)(2n-1)} \right]^{\frac{1}{2}} \exp(-\tfrac{1}{2}\beta\rho) (\beta\rho)^{|l|}$$

$$\times \ _1F_1(-n+|l|+1; \ 2|l|+1; \ \beta\rho) ; \ \beta = \frac{2\alpha}{a_o}$$

n	l	$R_{nl}(o)$
1	0	$R_{10}(\rho) = \beta \exp(-\frac{\beta\rho}{2}) = (\frac{Z}{a_o}) 4\exp(-\frac{2Z\rho}{a_o})$
2	0	$R_{20}(\rho) = \frac{\beta}{\sqrt{3}}(1-\beta\rho)\exp(-\frac{\beta\rho}{2}) = (\frac{Z}{a_o})\frac{4\sqrt{3}}{27} \left[3-4(\frac{Z\rho}{a_o})\right] \exp(-\frac{2Z\rho}{3a_o})$
2	1, -1	$R_{2\pm1}(\rho) = \frac{\beta}{\sqrt{6}}(\beta\rho)\exp(-\frac{\beta\rho}{2}) = (\frac{Z}{a_o})\frac{8\sqrt{6}}{27}(\frac{Z\rho}{a_o})\exp(-\frac{2Z\rho}{3a_o})$
3	0	$R_{30}(\rho) = \begin{cases} \frac{\beta}{2\sqrt{5}}\left[2 - 4\beta\rho + (\beta\rho)^2\right]\exp(-\frac{\beta\rho}{2}) \\ (\frac{Z}{a_o})\frac{4\sqrt{5}}{625}\left[25 - 40(\frac{Z\rho}{a_o}) + (\frac{Z\rho}{a_o})^2\right]\exp(-\frac{2Z\rho}{5a_o}) \end{cases}$
3	1, -1	$R_{3\pm1}(\rho) = \begin{cases} \frac{\beta}{\sqrt{30}}\left[3(\beta\rho) - (\beta\rho)^2\right]\exp(-\frac{\beta\rho}{2}) \\ (\frac{Z}{a_o})\frac{8\sqrt{30}}{1875}\left[15(\frac{Z\rho}{a_o}) - 4(\frac{Z\rho}{a_o})^2\right]\exp(-\frac{2Z\rho}{5a_o}) \end{cases}$
3	2, -2	$R_{3\pm2}(\rho) = \frac{\beta}{2\sqrt{30}}(\beta\rho)^2\exp(-\frac{\beta\rho}{2}) = (\frac{Z}{a_o})\frac{16\sqrt{30}}{1875}(\frac{Z\rho}{a_o})^2\exp(-\frac{2Z\rho}{5a_o})$
4	0	$R_{40}(\rho) = \begin{cases} \frac{\beta}{6\sqrt{7}}\left[6 - 18(\beta\rho) + 9(\beta\rho)^2 - (\beta\rho)^3\right]\exp(-\frac{\beta\rho}{2}) \\ (\frac{Z}{a_o})\frac{4\sqrt{7}}{50421}\left[1029-1764(\frac{Z\rho}{a_o})+504(\frac{Z\rho}{a_o})^2-32(\frac{Z\rho}{a_o})^3\right]\exp(-\frac{2Z\rho}{7a_o}) \end{cases}$
4	1, -1	$R_{4\pm1}(\rho) = \begin{cases} \frac{\beta}{4\sqrt{21}}\left[12(\beta\rho) - 8(\beta\rho)^2 + (\beta\rho)^3\right]\exp(-\frac{\beta\rho}{2}) \\ (\frac{Z}{a_o})\frac{16\sqrt{21}}{50421}\left[147(\frac{Z\rho}{a_o})-56(\frac{Z\rho}{a_o})^2+4(\frac{Z\rho}{a_o})^3\right]\exp(-\frac{2Z\rho}{7a_o}) \end{cases}$
4	2, -2	$R_{4\pm2}(\rho) = \begin{cases} \frac{\beta}{2\sqrt{210}}\left[5(\beta\rho)^2 - (\beta\rho)^3\right]\exp(-\frac{\beta\rho}{2}) \\ (\frac{Z}{a_o})\frac{16\sqrt{210}}{252105}\left[35(\frac{Z\rho}{a_o})^2 - 4(\frac{Z\rho}{a_o})^3\right]\exp(-\frac{2Z\rho}{7a_o}) \end{cases}$
4	3, -3	$R_{4\pm3}(\rho) = \frac{\beta}{12\sqrt{35}}(\beta\rho)^3\exp(-\frac{\beta\rho}{2}) = (\frac{Z}{a_o})\frac{64\sqrt{35}}{252105}(\frac{Z\rho}{a_o})^3\exp(-\frac{2Z\rho}{7a_o})$

FIGURE 3.2 The normalized radial functions, $R_{nl}(\rho)$, multiplied by Bohr radius a_o for nonrelativistic two-dimensional hydrogen atom (Z=1). The radius is measured here in units of a_o.

The radial functions $R_{nl}(\rho)$, Eq.(3.43b), indicate that, using the three dimensional hydrogen atom as a reference, the electron distribution is displaced towards the nucleus.

3.1.5 Radial Probability Distribution : The probability of finding the electron between ρ and $\rho + d\rho$ is equal to $w_{nl}(\rho)d\rho$ where

$$w_{nl}(\rho) = \rho[R_{nl}(\rho)]^2 \tag{3.48}$$

are the so-called radial probability distributions. These radial probability distributions have maxima that shift to large values of ρ as the quantum number n increases. Figures 3.3 illustrate this for the states listed in Table 3.1, whose the radial functions are shown in Figures 3.2. For the ground state, the radial probability distribution $w_{10}(\rho)$ has its maximum at ρ equal to (1/4) of the Bohr radius (a_o), while the three dimensional radial probability distribution peaks at the Bohr radius. This result is consistent with the result obtained before that the energy levels are lower in the planar cases.
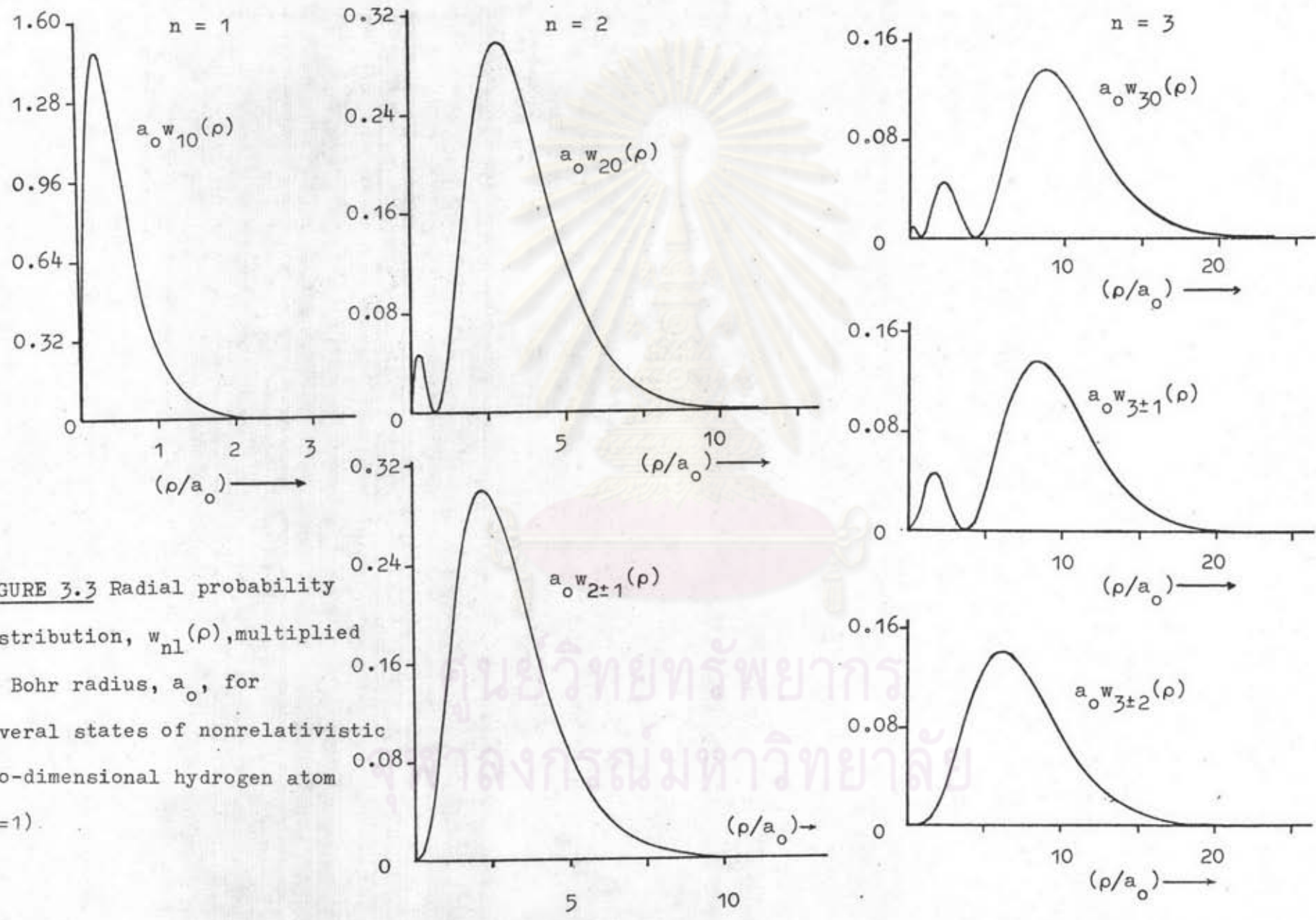
FIGURE 3.3 Radial probability distribution, $w_{nl}(\rho)$, multiplied by Bohr radius, a_o, for several states of nonrelativistic two-dimensional hydrogen atom $(Z=1)$.

3.1.6 Constant of the Motion and Interpretation of the Quantum
Numbers : Since the electron is confined to move only in a plane,
say, the xy-plane, only the z-component of the angular momemtum
exists ;

$$\vec{L} = \vec{r} \times \vec{p} = \hat{z} L_z \qquad (3.49)$$

In the plane polar coordinates (ρ, ϕ), this operator takes the form

$$L_z = -i\hbar \frac{\partial}{\partial \phi} \qquad (3.50)$$

Since L_z commutes with the Harmiltonian H , $[L_z, H] = 0$, we conclude
that L_z and H can have the simultaneous eigenfunctions and that L_z
is a constant of the motion. The eigenvalues of L_z can be obtained
by operating on the wave functions $U_{nl}(\rho, \phi)$ the operator in Eq.(3.50).
The result is

$$L_z U_{nl}(\rho, \phi) = l\hbar U_{nl}(\rho, \phi) , \qquad (3.51)$$

that is, the eigenvalues of L_z are $l\hbar$. It can be easily seen from
Eq.(3.51) that the eigenvalues of L^2 $(=L_z^2)$ are $(l\hbar)^2$. Thus, the
quantum number l tells us both the magnitude and direction of the
orbital angular momentum of the electron in the two dimensional
hydrogen atom.

By comparing the energy eigenvalues, the eigenvalues of the
z-component of the orbital angular momentum, and the magnitude of
the orbital angular momentum for the nonrelativistic two dimensional
hydrogen atom with those for the nonrelativistic three dimensional
hydrogen atom , see Table 3.2, we can conclude that the quantum
numbers n, |l|, and l are the two dimensional analog of the three
dimensional "principal", "orbital", and "magnetic orbital" quantum

numbers, respectively.

It is convenient at this point to introduce the nonrelativistic "two dimensional" spectroscopic notation by which the quantum states of the electron (without spin) are specified. The state of the electron is identified by writing the value of n, followed by the letter identifying $|l|$:

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

The value of l is also added to the symbol as a subscript. Thus, for example, the state belonging to n = 3, l = -1 is written as $3P_{-1}$.

In the next two sections, we will extend the Schroedinger wave mechanical treatment to include the effect of the electron spin and the effect due to the relativistic variation of mass with velocity, Sections 3.2 and 3.3 respectively.

TABLE 3.2 Comparision of some quantities for the nonrelativistic

two and three dimensional hydrogen atoms

Quantities	Two Dimensional Hydrogen Atom	Three Dimensional Hydrogen Atom
Energy eigenvalues	$E_n = -\dfrac{mZ^2e^4}{2\hbar^2(n-\frac{1}{2})^2}$ $n = 1, 2, 3, 4, \ldots$	$E_n = -\dfrac{mZ^2e^4}{2\hbar^2n^2}$ $n = 1, 2, 3, 4, \ldots$ (principal quantum number)
Magnitude of the orbital angular momentum	$|l|\,\hbar$ for a given n : $|l| = 0, 1, \ldots, (n-1)$	$\hbar\sqrt{l(l+1)}$ for a given n : $l = 0, 1, \ldots, (n-1)$ (orbital quantum number)
Eigenvalues of the z-component of the orbital angular momentum	$l\hbar$ for a given n : $l = 0, \pm1, \ldots, \pm(n-1)$ for a given $|l|$: $l = \pm|l|$	$m_l\hbar$ for a given n : $m_l = 0, \pm1, \ldots, \pm(n-1)$ for a given l : $m_l = 0, \pm1, \ldots, \pm l$ (magnetic orbital quantum number)

3.2 NONRELATIVISTIC TREATMENT OF THE ELECTRON SPIN FOR THE TWO DIMENSIONAL HYDROGEN ATOM.

In this section we will extend the Schrödinger wave mechanical treatment of the two dimensional hydrogen atom discussed in the preceeding section, in the same way as Pauli had been done for the three dimensional cases (21,39), to include the effect of the electron spin.

When taking into account the effect of the electron spin, the total energy of the electron in the two dimensional hydrogen atom consists of three parts : the kinetic energy, the electrostatic potential energy, and the energy due to the interaction of the electron's spin magnetic moment ($-\frac{e\vec{S}}{mc}$) with its orbital magnetic moment ($-\frac{e\vec{L}}{2mc} = -\frac{eL_z}{2mc}\hat{z}$) - the so-called spin-orbit interaction. The last part is (40)

$$H_{sp} = \frac{Ze^2}{2m^2c^2\rho^3} L_z S_z = \frac{\hbar Ze^2}{4m^2c^2\rho^3} L_z \sigma_z^P = \xi(\rho) L_z \sigma_z^P \qquad (3.52)$$

where $S_z = \frac{1}{2}\hbar\sigma_z^P$, σ_z^P is the Pauli matrix

$$\sigma_z^P = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

and

$$\xi(\rho) = \frac{\hbar Ze^2}{4m^2c^2\rho^3} \qquad (3.53)$$

The Hamiltonian operator is then

$$H = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi} \right) - \frac{Ze^2}{\rho} + H_{sp} \quad . \qquad (3.54)$$

3.2.1 <u>Constant of Motion</u> : The operators L_z, S_z, and $J_z = L_z + S_z$ commute with the Hamiltonian (3.54) and constitute a set of commuting constants of the motion, i.e., commute with each other. In computing the eigenvalues of the Hamiltonian (3.54) we therefore may restrict ourselves to the eigenfunctions that are the simultaneous eigenfunctions of L_z, S_z, and J_z.

3.2.2 <u>The Simultaneous Eigenfunctions of L_z, S_z, and J_z</u> : If we denote the eigenvalues of L_z by $l\hbar$ then the eigenvalue equation for L_z takes the form

$$L_z U_1(\rho,\phi) = \begin{bmatrix} -i\hbar \frac{\partial}{\partial\phi} & 0 \\ \\ 0 & -i\hbar \frac{\partial}{\partial\phi} \end{bmatrix} U_1(\rho,\phi) = l\hbar \, U_1(\rho,\phi) \quad . \quad (3.55)$$

The eigenfunction of L_z belonging to the eigenvalue $l\hbar$ is thus

$$U_1(\rho,\phi) = \begin{bmatrix} R_1(\rho)e^{il\phi} \\ \\ R_2(\rho)e^{il\phi} \end{bmatrix} \quad , \quad (3.56)$$

where, in order to assure single-valueness of $U_1(\rho,\phi)$, l is restricted to the values $0, \pm 1, \pm 2, \pm 3, \ldots$.

By writing

$$U_1^A(\rho,\phi) = \begin{bmatrix} R_1(\rho)e^{il\phi} \\ \\ 0 \end{bmatrix} \text{ and } U_1^A(\rho,\phi) = \begin{bmatrix} 0 \\ \\ R_2(\rho)e^{il\phi} \end{bmatrix} \quad (3.57)$$

and operating on each of these U's the operator

$$J_z = \begin{bmatrix} -i\hbar \frac{\partial}{\partial\phi} + \tfrac{1}{2}\hbar & 0 \\ \\ 0 & -i\hbar \frac{\partial}{\partial\phi} - \tfrac{1}{2}\hbar \end{bmatrix} \quad (3.58)$$

we find that

$$J_z U_1^A(\rho,\phi) = (1+\tfrac{1}{2})\hbar U_1^A(\rho,\phi) \qquad (3.59)$$

and

$$J_z U_1^B(\rho,\phi) = (1-\tfrac{1}{2})\hbar U_1^B(\rho,\phi) \qquad (3.60)$$

so that $U_1^A(\rho,\phi)$ and $U_1^B(\rho,\phi)$ are the eigenfunctions of J_z belonging to the eigenvalues $j\hbar=(1+\tfrac{1}{2})\hbar$ and $j\hbar=(1-\tfrac{1}{2})\hbar$, respectively. Thus, there exists two sets of functions which are simultaneous eigenfunctions of J_z and L_z ; namely

$$U_{1,j=1+\frac{1}{2}}^{A} (\rho,\phi) = \begin{bmatrix} R_1(\rho)e^{il\phi} \\ \\ 0 \end{bmatrix} \qquad (3.61)$$

and

$$U_{1,j=1-\frac{1}{2}}^{B} (\rho,\phi) = \begin{bmatrix} 0 \\ \\ R_2(\rho)e^{il\phi} \end{bmatrix} . \qquad (3.62)$$

$U_{1,j=1+\frac{1}{2}}^{A}$ is also the eigenfunction of S_z belonging to the eigenvalue $\tfrac{1}{2}\hbar$ and therefore corresponds to the spin-up case, where as $U_{1,j=1-\frac{1}{2}}^{B}$ corresponds to the spin-down case.

Thus, instead of treating the eigenvalue equation $HU = EU$ in its generality, we restrict ourselves to the simpler problem of studying separately the two equations

$$H \, U_{1,j=1+\frac{1}{2}}^{A} (\rho,\phi) = E \, U_{1,j=1+\frac{1}{2}}^{A} (\rho,\phi) \qquad (3.63)$$

and

$$H \, U_{1,j=1-\frac{1}{2}}^{B} (\rho,\phi) = E \, U_{1,j=1-\frac{1}{2}}^{B} (\rho,\phi) \qquad (3.64)$$

where H is the Hamiltonian given in Eq.(3.54). Substituting Eqs.(3.61) and (3,62) into Eqs.(3.63), we obtain, after some simple algebra, the two radial equations :

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} + \frac{2m}{\hbar^2}\left(E + \frac{Ze^2}{\rho}\right) - \frac{1^2}{\rho^2} - \frac{2ml}{\hbar}\xi(\rho) \right] R_1(\rho) = 0 \qquad (3.65)$$

and

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} + \frac{2m}{\hbar^2}\left(E + \frac{Ze^2}{\rho}\right) - \frac{1^2}{\rho^2} + \frac{2ml}{\hbar}\xi(\rho) \right] R_2(\rho) = 0 \qquad (3.66)$$

Apart from the terms in $\xi(\rho)$, Eqs.(3.65) and (3.66) are both identical with the Schroedinger radial equation (3.5).

3.2.3 The Spin Correction : Since spin effects are known to be small, we may consider the terms in $\xi(\rho)$ as perturbing potentials and may handle Eqs.(3.65) and (3.66) by perturbation method .(36). In the zeroth approximation, the energy eigenvalues are

$$E_n^{(0)} = -\frac{mZ^2e^4}{2\hbar^2(n-\frac{1}{2})^2} \quad , \quad n = 1, 2, 3,\ldots, \tag{3.67}$$

and the corresponding spin-up and spin-down normalized eigenfunctions are

$$U_{nlj}^{A(0)}(\rho,\phi) = R_{nl}(\rho)\,\phi_1(\phi)\begin{pmatrix}1\\0\end{pmatrix} \quad , \tag{3.68}$$

$$U_{nlj}^{B(0)}(\rho,\phi) = R_{nl}(\rho)\,\phi_1(\phi)\begin{pmatrix}0\\1\end{pmatrix} \quad , \tag{3.69}$$

where $R_{nl}(\rho)$ and $\phi_1(\phi)$ are given in Eqs.(3.43b) and (3.43c).

The first-order energy correction due to the spin-orbit interaction for the spin-up case is

$$E_{n\,sp.}^{A(1)} = \int_0^\infty \int_0^{2\pi} [U_{nlj}^{A(0)}(\rho,\phi)]^\dagger H_{sp} U_{nlj}^{A(0)}(\rho,\phi)\,d\phi\,\rho d\rho . \tag{3.70}$$

Since

$$H_{sp}U_{nlj}^{A(0)}(\rho,\phi) = \frac{Ze^2\hbar^2 l}{4m^2c^2\rho^3} U_{nlj}^{A(0)}(\rho,\phi) , \tag{3.71}$$

Eq.(3.70) then becomes

$$E_{n\,sp.}^{A(1)} = \frac{Ze^2\hbar^2 l}{4m^2c^2}\int_0^\infty\int_0^{2\pi}[U_{nlj}^{A(0)}(\rho,\phi)]^\dagger\frac{1}{\rho^3}U_{nlj}^{A(0)}(\rho,\phi)\,d\phi\,\rho d\rho$$

$$= \frac{Ze^2\hbar^2 l}{4m^2c^2}\left\langle\rho^{-3}\right\rangle . \tag{3.72}$$

From Appendix A, the expectation value of ρ^{-3} is

From Appendix A, the expectation value of ρ^{-3} is

$$\langle \rho^{-3} \rangle = \frac{m^3 Z^3 e^6}{\hbar^6 (n-\frac{1}{2})^3 |l| (|l|-\frac{1}{2})(|l|+\frac{1}{2})} \qquad , \qquad (3.73)$$

we thus get

$$E_{\substack{nl \\ sp.}}^{A(1)} = \frac{mZ^4 e^8}{4\hbar^4 c^2 (n-\frac{1}{2})^3} \frac{1}{|l|(|l|-\frac{1}{2})(|l|+\frac{1}{2})} \qquad . \qquad (3.74)$$

In a similar way, the first-order energy correction for the spin-down case is found to be

$$E_{\substack{nl \\ sp.}}^{B(1)} = -\frac{mZ^4 e^8}{4\hbar^4 c^2 (n-\frac{1}{2})^3} \frac{1}{|l|(|l|-\frac{1}{2})(|l|+\frac{1}{2})} \qquad . \qquad (3.75)$$

To the first-order approximation, the eigenvalues for the spin-up and spin-down cases are then

$$E_{nl}^{A(1)} = E_n^{(0)} + E_{\substack{nl \\ sp.}}^{A(1)} \qquad \text{and} \qquad E_{nl}^{B(1)} = E_n^{(0)} + E_{\substack{nl \\ sp.}}^{B(1)} \qquad , \qquad (3.76)$$

respectively. From Eqs.(3.76) it follow that the states with positive l and spin-up have the same energy levels as those with negative l and spin-down;

$$E_{n+}^{A(1)} = E_{n-}^{B(1)} = -\frac{mZ^2 e^4}{2\hbar^2 (n-\frac{1}{2})^2} + \frac{mZ^4 e^8}{4\hbar^4 c^2 (n-\frac{1}{2})^3} \frac{1}{(|l|-\frac{1}{2})(|l|+\frac{1}{2})} \quad .(3.77)$$

Also, the states with negative l and spin-up have the same energy levels as the states with positive l and spin-down;

$$E_{n-}^{A(1)} = E_{n+}^{B(1)} = -\frac{mZ^2 e^4}{2\hbar^2 (n-\frac{1}{2})^2} - \frac{mZ^4 e^8}{4\hbar^4 c^2 (n-\frac{1}{2})^3} \frac{1}{(|l|-\frac{1}{2})(|l|+\frac{1}{2})} \quad .(3.78)$$

These results are the expected ones since, in this case, there is no distinction between up- and down-directions in the space.

The levels (3.77) and (3.78) are shown in Figure 3.4 for Z=45.*

It is important to note that, from Eq.(3.52), the spin-orbit interaction energy is zero whenever l=0, the spin thus causes no displacement in the energy levels of the states in which l=0. This conclusion is borne out by Eqs.(3.65) and (3.66), which become identical with the Schroedinger radial equation (3.5) when l=0.

However Eqs.(3.77) and (3.78) give nonvanishing spin corrections even when l=0. The answer to this contradiction lies in the fact that the average value of ρ^{-3} given by Eq.(3.73) contains the factor |l| in the denominator, and that in getting the corrections (3.77) and (3.78) we have cancelled this |l| with the l that multiplies $\mathfrak{s}(\rho)$ in Eqs.(3.65) and (3.66)

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* For Z = 1 the splitting of the energy levels are so small that it is inconvenient to represent them graphically.

3.3 RELATIVISTIC CORRECTIONS

The starting point of nonrelativistic Schroedinger's wave mechanics consists in writing the classical expression for the Hamiltonian H, which is defined as the sum of the kinetic energy T and the potential energy V. That is

$$H = T + V = \frac{p^2}{2m} + V \qquad (3.79)$$

This equation is not relativistically correct since in the special theory of relativity the kinetic energy of the particle is the difference between its energy at momentum p and its rest energy mc^2;

$$T_{rel} = (c^2p^2 + m^2c^4)^{1/2} - mc^2 \quad , \qquad (3.80)$$

where m is the rest mass of the particle. The relativistically correct expression for the Hamiltonian is then

$$H_{rel} = T_{rel} + V = mc^2\left[(1 + \frac{p^2}{m^2c^2})^{1/2} - 1\right] + V \quad . \qquad (3.81)$$

In the nonrelativistic limit, $v \ll c$ or $p \ll mc$, the above relation can be written approximately as

$$H_{rel} = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + V \qquad (3.82)$$

where we have taken only the first three terms in the binomial expansion of $(1 + \frac{p^2}{m^2c^2})^{1/2}$ .Comparing this with Eq.(3.79), we see that the error in the classical expression for the Hamiltonian is, to the first-order approximation,

$$H_{rel} = -\frac{p^4}{8m^3c^2} = -\frac{T^2}{2mc^2} = -\frac{(E-V)^2}{2mc^2} \quad , \qquad (3.83)$$

where $E = E_n$ is the energy eigenvalue derived from the nonrelativistic Schroedinger wave mechanics.

In the case of the two dimensional hydrogen atom, if we use the eigenfunctions (3.68) and (3.69) as the unperturbed eigenfunctions, we can use the non-degenerate perturbation theory to evaluate the shift in the energy levels of the corresponding states due to the addition of the term H_{rel}. According to the theory, the first-order energy correction is

$$E_{\substack{n\\rel}}^{(1)} = -\frac{1}{2mc^2}\int_0^\infty\int_0^{2\pi}\left[U_{nlj}^{(0)}(\rho,\phi)\right]^\dagger(E_n^2 + V^2 - 2E_n V)U_{nlj}^{(0)}(\rho,\phi)\,d\phi\,\rho\,d\rho. \tag{3.84}$$

Now

$$V(\rho) = -\frac{Ze^2}{\rho} \quad\text{and}\quad E_n = E_n^{(0)} = -\frac{mZ^2e^4}{2\hbar^2(n-\frac{1}{2})^2}, \tag{3.85}$$

so we obtain

$$E_{\substack{n\\rel}}^{(1)} = -\frac{mZ^4e^8}{8\hbar^4c^2(n-\frac{1}{2})^4} - \frac{Z^2e^4}{2mc^2}\left\langle\rho^{-2}\right\rangle + \frac{Z^3e^6}{2\hbar^2c^2(n-\frac{1}{2})^2}\left\langle\rho^{-1}\right\rangle. \tag{3.86}$$

Since, from Appendix A,

$$\left\langle\rho^{-1}\right\rangle = \frac{mZe^2}{\hbar^2(n-\frac{1}{2})^2} \quad\text{and}\quad \left\langle\rho^{-2}\right\rangle = \frac{m^2Z^2e^4}{\hbar^4(n-\frac{1}{2})^3|1|}, \tag{3.87}$$

Eq.(3.86) becomes

$$E_{\substack{nl\\rel}}^{(1)} = -\frac{mZ^4e^8}{2\hbar^4c^2(n-\frac{1}{2})^3}\left[\frac{1}{|1|} - \frac{3}{4}\left(\frac{1}{n-\frac{1}{2}}\right)\right]. \tag{3.88}$$

Eq.(3.88) gives the energy corrections due to the relativistic effect for the states in which $1 \neq 0$. (see Figure 3.4) For the states with $1 = 0$, the expectation value of ρ^{-2} diverges, and hence, it is impossible to evaluate the energy corrections due to the relativistic effect for these states by mean of the perturbation method.

As in the case of the three dimensional hydrogen atom, there is another relativistic correction term - the two dimensional analog of the three dimensional "Darwin" term - whose the existence cannot be predicted since it has no classical counter part (see Appendix B):

$$H_{Darwin} = -\frac{Ze^2\hbar^2}{8m^2c^2}\frac{1}{\rho^3}. \tag{3.89}$$

This term contributes to the energy levels E_n the amount

$$E_{Darwin}^{(1)} = \left\langle H_{Darwin} \right\rangle = -\frac{Ze^2\hbar^2}{8m^2c^2}\left\langle \rho^{-3} \right\rangle$$

$$= -\frac{mZ^4e^8}{2\hbar^4c^2(n-\frac{1}{2})^3}\frac{1}{4|l|(|l|-\frac{1}{2})(|l|+\frac{1}{2})} \ , \ l\neq 0. \quad (3.90)$$

Thus, when taking into account the effects due to the spin-orbit interaction, the relativistic variation of mass with velocity, and the two dimensional Darwin term, the energy levels for the two dimensional hydrogen atom are, to the first-order approximation,

$$E_{nk}^{(1)} = E_n^{(0)} + E_{nk\atop sp}^{(1)} + E_{nk\atop rel}^{(1)} + E_{Darwin}^{(1)}$$

$$= -\frac{mZ^2e^4}{2\hbar^2(n-\frac{1}{2})^2} - \frac{mZ^4e^8}{2\hbar^4c^2(n-\frac{1}{2})^4}\left[\frac{(n-\frac{1}{2})}{|k|} - \frac{3}{4}\right], \ l\neq 0 \quad (3.91)$$

where k is the new quantum number defined by the relations

$$k = \begin{cases} -j & \text{for} \quad j = l + \frac{1}{2} \ (\text{spin-up}) \\ j & \text{for} \quad j = l - \frac{1}{2} \ (\text{spin-down}) \end{cases} \quad (3.92)$$

Equation (3.91) predicts exactly the same energy levels for the two dimensional hydrogen atom as those predicted by the Dirac relativistic quantum mechanics (Chapter IV) provided that this equation is extended to be valid for the states in which $l = 0$.
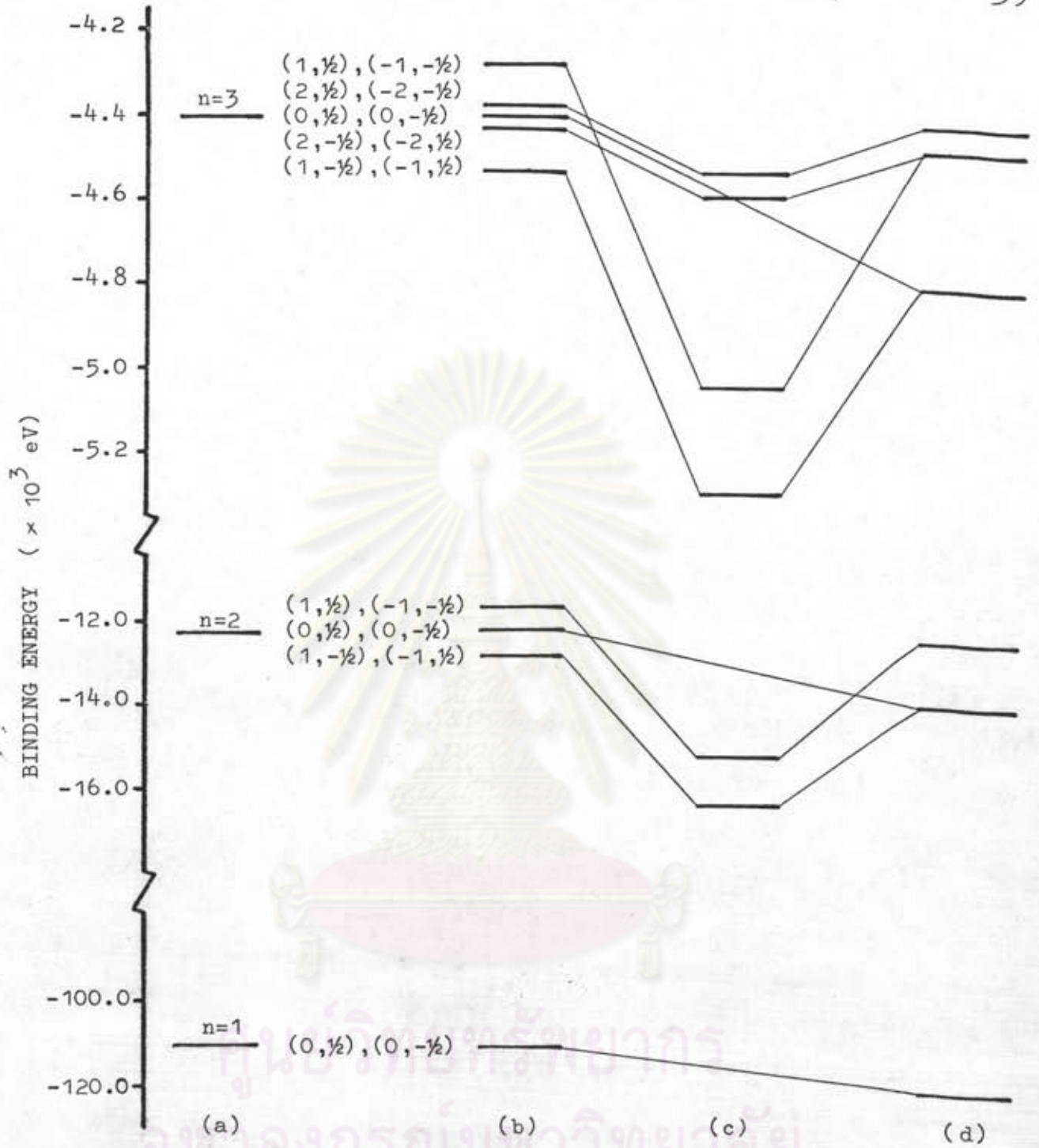
FIGURE 3.4 Energy levels of the nonrelativistic hydrogen atom (2D) after taken into account the spin-and-relativistic effects : (a) nonrelativistic energy levels for Z=45, (b) with spin-orbit interaction, (c) with spin-orbit interaction and relativistic variation of mass , (d) with spin-orbit interaction, relativistic variation of mass, and two-dimensional Darwin term.