CHAPTER V

CONCLUSION AND DISCUSSION

The problem of the two dimensional hydrogen atom, which is defined to be a system in which the motion of the electron around the nucleus under the influence of an attractive Coulomb potential is constrainted to be planar, was studied both by means of the Schroedinger nonrelativistic wave mechanics with the extension to include the effects of the electron spin and the relativistic variation of mass with velocity (Chapter III), and by the Dirac relativistic wave mechanics (Chapter IV). As in the case of the three dimensional hydrogen atom, the results obtained from these two methods are consistent, i.e., in the nonrelativistic limit the results obtained from the Dirac wave mechanics reduce to those obtained from the Schroedinger wave mechanics.

According to the Schroedinger wave mechanics, the energy levels of the electron are

$$E_n = - \frac{mZ^2e^4}{2\hbar^2(n - \frac{1}{2})^2} \quad , n = 1, 2, 3, \cdots , \qquad (3.31)$$

which indicate that, using the three dimensional hydrogen atom as reference, the energy levels are lower in the planar case . The normalized wave functions which correspond to the energy eigenvalues (3.31) are

$$U_{n1}(\rho,\phi) = R_{n1}(\rho)\, \Phi_1(\phi) , \qquad (3.43a)$$

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

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

$$\phi_l(\phi) = \frac{1}{\sqrt{2\pi}}\exp(il\phi)\ , \qquad (3.43c)$$

where β is defined by the relation

$$\beta = \frac{4Z}{a_o(2n - 1)}\ . \qquad (3.44)$$

In consistent with the lower value of the energy levels, it follows from the form of the wave functions that the electron distribution is displaced toward the nucleus. The energy eigenvalues (3.31) depend only on the quantum number n and so are degenerate with respect to the quantum number l . Since for each value of n, l can vary from -(n-1) to (n-1) , the total degeneracy of the energy level E_n is then (2n-1). (In the three dimensional hydrogen atom , the total degeneracy of the energy level E_n is n^2).

If the effect of the electron spin and the relativistic variation of mass with velocity are taken into account , the energy levels for the states with $l \neq 0$ can be found by using the perturbation method. To the first order approximation, the energy level of the electron are

$$E_{nl}^{(1)} = -\frac{mZ^2e^4}{2\hbar^2(n-\frac{1}{2})^2} - \frac{mZ^4e^8}{2\hbar^4c^2(n-\frac{1}{2})^3}\left\{\frac{2(|l|-\frac{1}{2})(|l|+\frac{1}{2})}{|l|(|l|-\frac{1}{2})(|l|+\frac{1}{2})}\frac{|l| \mp 1}{2}\right.$$

$$\left. - \frac{3}{4(n-\frac{1}{2})}\right\}\ ,$$

where the upper and lower signs stand for the spin-up and spin-

down states, respectively.

If, in addition to the effects of the electron spin and the relativistic variation of mass, the effect of the two dimensional Darwin term (see Appendix B)

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

was also taken into account , the energy levels of the electron for the states in which $l \neq 0$ are then

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

where k is the new quantum number defined by the relation

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

The perturbation method is not applicable to the states with $l = 0$ because in evaluating the energy shifts due to the relativistic variation of mass and the two dimensional Darwin term we deal with the expectation values of ρ^{-2} and ρ^{-3} , respectively, which are not finite for $l = 0$. (In the three dimensional hydrogen atom, the expectation values of r^{-n} are not finite for $n \geqslant 3$.) However, Eq.(3.91) gives the finite energy levels even for the states with $l = 0$. If we extend Eq.(3.91) to be valid for the states with $l = 0$ as well , then it can be shown that the energy levels of the electron predicted by the Schroedinger wave mechanics are consistent with those predicted by the Dirac relativistic wave mechanics.

When the two dimensional hydrogen atom problem is solved by means of the Dirac relativistic wave mechanics, the energy levels of the electron turn out to be

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

and the corresponding normalized wave functions are, as in the case of the relativistic three dimensional hydrogen atom, divided into two classes ;

(a) for the spin-up states

$$U^{A}_{njk}(\rho,\phi) = \begin{bmatrix} R^{1}_{nk}(\rho)\ \phi^{1}_{j}(\phi) \\ 0 \\ 0 \\ -iR^{4}_{nk}(\rho)\ \phi^{2}_{j}(\phi) \end{bmatrix} , \quad (4.152)$$

and (b) for the spin-dowm states

$$U^{B}_{njk}(\rho,\phi) = \begin{bmatrix} 0 \\ R^{1}_{nk}(\rho)\ \phi^{2}_{j}(\phi) \\ -iR^{4}_{nk}(\rho)\ \phi^{1}_{j}(\phi) \\ 0 \end{bmatrix} , \quad (4.153)$$

where

$$R^{1}_{nk}(\rho) = -\left\{ \frac{(\lambda_{nk})^2 \Gamma(\bar{n}+2\gamma_k+1)}{N_{nk}(N_{nk}-k)\left[\Gamma(2\gamma_k+1)\right]^2 \bar{n}!} \right\}^{\frac{1}{2}} (2\lambda_{nk}\rho)^{\gamma_k - \frac{1}{2}} \exp(-\lambda_{nk}\rho)$$

$$(1+\epsilon_{nk})^{\frac{1}{2}} \left\{ \bar{n}\ {}_1F_1(-\bar{n}+1;2\gamma_k+1;2\lambda_{nk}\rho) \right.$$

$$\left. - (N_{nk}-k)\ {}_1F_1(-\bar{n};2\gamma_k+1;2\lambda_{nk}\rho) \right\} , \quad (4.154)$$

$$R^{4}_{nk}(\rho) = -\left\{\frac{(\lambda_{nk})^{2}\Gamma(\bar{n}+2\gamma_{k}+1)}{N_{nk}(N_{nk}-k)[\Gamma(2\gamma_{k}+1)]^{2}\,\bar{n}!}\right\}^{\frac{1}{2}} (2\lambda_{nk}\rho)^{\gamma_{k}-\frac{1}{2}} \exp(-\lambda_{nk}\rho)$$

$$(1-\epsilon_{nk})^{\frac{1}{2}}\left\{\bar{n}\ {}_{1}F_{1}(-\bar{n}+1;2\gamma_{k}+1;2\lambda_{nk}\rho)\right.$$

$$\left. + (N_{nk}-k)\ {}_{1}F_{1}(-\bar{n};2\gamma_{k}+1;2\lambda_{nk}\rho)\right\}, \qquad (4.155)$$

$$\phi^{1}_{j}(\phi) = \frac{1}{\sqrt{2\pi}} \exp(i[j-\tfrac{1}{2}]\phi) \quad , \qquad (4.42)$$

and

$$\phi^{2}_{j}(\phi) = \frac{1}{\sqrt{2\pi}} \exp(i[j+\tfrac{1}{2}]\phi) \quad . \qquad (4.43)$$

For a given value of the quantum number n, there are n possible values of $|k|$ and therefore n different values of E_{nk} for each n . The complete degeneracy of a given n in the nonrelativistic case is then lifted by relativistic effects. However, there still remains a degeneracy of the states with same n and $|k|$ but differ in k, j, or l. The relationship between the relativistic and the nonrelativistic energy eigenvalues can be seen by expanding Eq.(4.103) in powers of $(Z\alpha)$. This procedure yields

$$E_{nk} = mc^{2} - \frac{mc^{2}(Z\alpha)^{2}}{2(n-\frac{1}{2})^{2}} - \frac{mc^{2}(Z\alpha)^{4}}{2(n-\frac{1}{2})^{4}}\left[\left(\frac{n-\frac{1}{2}}{k}\right) - \frac{3}{4}\right] - \mathcal{O}(Z\alpha)^{6} \quad . \qquad (4.174)$$

The first term is the rest energy of the electron. The second term is the nonrelativistic energy. The terms in $(Z\alpha)^{4}$ are exactly what is obtained in the nonrelativistic theory if the first order perturbation calculation is used to evaluate the contribution of the sum of the following three terms :

(i) the additional energy due to the relativistic variation of mass ;

(ii) the spin - orbit interaction ;

(iii) the two dimensional 'Darwin' term .

In the nonrelativistic limit, the relativistic radial functions can be shown to reduce to the nonrelativistic ones. In such limit, the small component (the last two components) vanishes and the large one reduces to the nonrelativistic radial function

$$R^{1}_{nk}(\rho) \xrightarrow[c\longrightarrow\infty]{\alpha\longrightarrow 0} \begin{cases} R_{nl}(\rho) & \text{for negative k} \\ -R_{nl}(\rho) & \text{for positive k} \end{cases} \qquad (4.166)$$

$$R^{4}_{nk}(\rho) \xrightarrow[c\longrightarrow\infty]{\alpha\longrightarrow 0} 0 \ .$$

Since the negative sign in (4.166) has no effect on the values of the physical observable quantities, it can be concluded that the results obtained from the relativistic and the nonrelativistic wave mechanics are consistent.

It is very interesting to note that the eigenvalues of the two dimensional hydrogen atom are very different from those of the three dimensional hydrogen atom. We all know that the quantum mechanical results for the eigenvalues of the nonrelativistic and the relativistic three dimensional hydrogen atoms are identical with the values predicted by the Bohr and the Sommerfeld theories, repectively. Since both the Bohr and the Sommerfeld theories involve a planar orbital motion, which is really a two dimensional motion, one might expect the Bohr result to agree with the quantum mechanical results for the nonrelativistic two dimensional hydrogen atom, and the Sommerfeld result to agree with

the relativistic one . The fact that these are not the cases, show even more convincingly the accidental nature of the coincidence between the Bohr result and the eigenvalues of the quantum mechanical nonrelativistic three dimensional hydrogen atom, and between the Sommerfeld result and the eigenvalues of the relativistic three dimensional hydrogen atom.

Recently, Bruce (53) has presented discussion of the relativistic two dimensional hydrogen atom but in his treatment the matrices α_x, α_y, and β are chosen to be 2-by-2 matrices, i.e.,

$$\alpha_x = \sigma_x^P \quad , \quad \alpha_y = \sigma_y^P \text{ , and } \quad \beta = \sigma_z^P \text{ ,} \tag{5.1}$$

where the matrices σ^P's are the Pauli spin matrices. As a result of this choice of α's and β, there exists only one constant of the motion, namely, the z-component of the total angular momentum

$$J_z = L_z + \frac{\hbar}{2}\sigma_z^P \text{ ,} \tag{5.2}$$

where as, in our treatment there are two commuting constants of the motion J_z and K ;

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

The wave functions in Bruce's treatment are thus not decomposed into two classes. Moreover, in Bruce's treatment, the positive energy solutions are associated only with spin up and negative energy with spin down. (In our treatment, the wave functions are decomposed into two classes, one corresponds to spin up and the other to spin down.) However, Bruce's results for the eigenvalues are identical with the values predicted by our treatment.