

Dirac equation's Mystery

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Abstract

Angular momentum j in the Dirac equation and j in the schringer equation are equal or different ? they are equal. but, $j = 0$ in the dirac equation is forbidden, $j = 0$ in the schringer equation is allowed. from this fact, it seems Dirac equation is not appropriate to study atomic phenomenon. maybe, only in a central field of force.

증명(proof)

수소원자(hydrogen)에 대한 Dirac equation [1]

$$\left(\frac{1}{a_1} - \frac{\alpha}{r}\right)\Psi_a - \left(\frac{\partial}{\partial r} + \frac{j+1}{r}\right)\Psi_b = 0$$

$$\left(\frac{1}{a_2} + \frac{\alpha}{r}\right)\Psi_b - \left(\frac{\partial}{\partial r} - \frac{j-1}{r}\right)\Psi_a = 0$$

위의 2개의 식을 행렬(matrix)로 표현해보면 이러하다.

| | | | | |
|---|---|---|----------|----------|
| $\left(\frac{1}{a_1} - \frac{\alpha}{r}\right)$ | $-\left(\frac{\partial}{\partial r} + \frac{j+1}{r}\right)$ | = | Ψ_a | 0 |
| $-\left(\frac{\partial}{\partial r} - \frac{j-1}{r}\right)$ | $\left(\frac{1}{a_2} + \frac{\alpha}{r}\right)$ | | | Ψ_b |

위의 matrix 에 크라머즈 룰(Cramer's Rule)을 적용하여 본다.

If $\Psi_a, \Psi_b \neq 0$, 행렬식(Determinant)은 0 이 되어야 한다.(Determinant = 0)

$$\left(\frac{1}{a_1} - \frac{\alpha}{r}\right)\left(\frac{1}{a_2} + \frac{\alpha}{r}\right) - \left(\frac{\partial}{\partial r} - \frac{j-1}{r}\right)\left(\frac{\partial}{\partial r} + \frac{j+1}{r}\right) = 0 \quad (1)$$

$$\left(\frac{1}{a_1} \frac{1}{a_2} + \left(\frac{1}{a_1} - \frac{1}{a_2}\right)\frac{\alpha}{r} - \frac{\alpha}{r} \frac{\alpha}{r}\right) - \left(\frac{\partial}{\partial r} \frac{\partial}{\partial r} - \frac{j-1}{r} \frac{\partial}{\partial r} + \frac{\partial}{\partial r} \frac{j+1}{r} - \left(\frac{j-1}{r}\right)\left(\frac{j+1}{r}\right)\right) = 0 \quad (2)$$

$$\left(\frac{1}{a_1} \frac{1}{a_2} + \left(\frac{1}{a_1} - \frac{1}{a_2}\right)\frac{\alpha}{r} - \frac{\alpha^2}{r^2}\right) - \left(\frac{\partial}{\partial r} \frac{\partial}{\partial r} - \frac{j-1}{r} \frac{\partial}{\partial r} - \frac{j+1}{r^2} + \frac{j+1}{r} \frac{\partial}{\partial r} - \left(\frac{j-1}{r}\right)\left(\frac{j+1}{r}\right)\right) = 0 \quad (3)$$

$$\left(\frac{1}{a_1} \frac{1}{a_2} + \left(\frac{1}{a_1} - \frac{1}{a_2}\right) \frac{\alpha}{r} - \frac{\alpha^2}{r^2}\right) - \left(\frac{\partial}{\partial r} \frac{\partial}{\partial r} - \frac{j-1}{r} \frac{\partial}{\partial r} + \frac{j+1}{r} \frac{\partial}{\partial r} - \frac{j+1}{r^2} - \left(\frac{j-1}{r}\right) \left(\frac{j+1}{r}\right)\right) \Psi = 0 \quad (4)$$

$$\left(\frac{1}{a_1} \frac{1}{a_2} + \left(\frac{1}{a_1} - \frac{1}{a_2}\right) \frac{\alpha}{r} - \frac{\alpha^2}{r^2}\right) - \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{j(j+1)}{r^2}\right) \Psi = 0 \quad (5)$$

Equation (5)에 Ψ 를 붙이면 아래와 같다.

$$\left(\left(\frac{1}{a_1} \frac{1}{a_2} + \left(\frac{1}{a_1} - \frac{1}{a_2}\right) \frac{\alpha}{r} - \frac{\alpha^2}{r^2}\right) - \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{j(j+1)}{r^2}\right)\right) \Psi = 0 \quad (6)$$

$$\left(\left(\frac{H^2 - m^2 c^4}{\hbar^2 c^2} + \frac{2H}{\hbar c} \frac{\alpha}{r} + \frac{\alpha^2}{r^2}\right) + \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{j(j+1)}{r^2}\right)\right) \Psi = 0$$

Equation (6) is the relativistic analogic Schrodinger' equation in a central field of force

여기서 if electron's velocity $v \ll c$ (light velocity), schrodinger equation is (7)

$$\left(\frac{2m}{\hbar} \left(H + \frac{e^2}{r}\right) + \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{j(j+1)}{r^2}\right)\right) \Psi = 0 \quad (7)$$

디랙방정식의 각운동량 j 와 슈뢰딩거 방정식의 궤도 각운동량 j 은 동일하다.

한편, 디랙방정식의 수소원자 에너지 준위(Energy levels of hydrogen atom)는 다음과 같다. [2]

$$\frac{H}{mc^2} = \left\{1 + \frac{\alpha^2}{(n + \sqrt{j^2 - \alpha^2})^2}\right\}^{-\frac{1}{2}} \quad (8)$$

$j = 0$ at the Dirac equation is forbidden

디랙방정식에서는 $j = 0$ 이면 에너지 준위(Energy levels)가 허수(imaginary number)를 갖는 반면

$j = 0$ at the schrodinger equation is allowed

슈뢰딩거 방정식은 $j = 0$ 은 당연한 것이며 S 오비탈(S orbital)을 가르킨다.

결론(conclusion)

j 가 반정수 $\frac{1}{2}, \frac{3}{2}, \dots$ 를 가질 가능성은 있는가. 그럴 수는 없다. 디랙방정식의 각운동량은

슈뢰딩거방정식의 궤도 각운동량과 동일한 것인데, 수소원자에 그런 상태가 존재하지 않는다.

아무래도 파동방정식이 2계 미분형식인 것과는 달리 디랙방정식이 공간에 대한 1계 미분형식이라 물질의 파동현상을 다루는데 불완전한 것 같다.

결론적으로 디랙방정식이 중심력장을 갖는 자연현상을 기술할 수 없음을 보여준다.

In conclusion, I think Dirac equation is not appropriate to study hydrogen atomic phenomenon.

Reference

[1] P.A.M. DIRAC, the Principles of Quantum Macanics 4th ed. (OXFORD AT THE CLAREN 1967), p.270

[2] P.A.M. DIRAC, the Principles of Quantum Macanics 4th ed. (OXFORD AT THE CLAREN 1967), p.272