THE RIGID ROTATOR ACCORDING TO
RELATIVISTIC QUANTUM MECHANICS

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Received September 22, 1964
(Communicated by Dr. K. S. Viswanathan, F.A.SC.)

After the classic application of the Relativistic Wave Equation of Dirac to the theory of hydrogen fine structure,1-3 there were several other applications of the equation to problems solved by non-relativistic Quantum Mechanics. Sauter4 treated the problem of a particle in a uniform field \( V(x) = ax \) and Nikolsky5 considered the problem of the harmonic oscillator with \( V(x) = \omega x^2 \). The general case when the potential \( V(x) \) is a polynomial of arbitrary degree in \( x \) or \( 1/x \) was treated by Plesset.6 However, the problem of the rigid rotator does not appear to have been considered and the purpose of this note is to determine the energy eigenvalues of a rigid rotator according to both the Klein-Gordon and Dirac equations.

For the sake of completeness, we first of all consider the rather trivial case of a single Klein-Gordon particle of rest mass \( m \) at a fixed distance \( 'a' \) from a centre of rotation with moment of inertia \( I = ma^2 \). The stationary states of this system must satisfy the Klein-Gordon equation,

\[
\nabla^2 \psi + \frac{1}{\hbar^2 c^2} (W^2 - \varepsilon^2) \psi = 0; \quad \varepsilon = mc^2; \quad \hbar = \frac{\hbar}{2m}
\]

which, in spherical co-ordinates with \( r = a \), becomes

\[
\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{1}{\hbar^2 \varepsilon} (W^2 - \varepsilon^2) \psi = 0.
\]

Comparing (2) with the corresponding non-relativistic Schrödinger equation, we immediately obtain

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\[ \frac{I}{\hbar^2} (W^2 - \varepsilon^2) = I (l + 1); \ l \ \text{integral} \]

from which follows

\[ W = W_l = \varepsilon \sqrt{1 + \frac{l(l + 1)}{I\varepsilon}}. \quad \text{(3)} \]

One observes that, with \( W = E + \varepsilon \), (3) goes over, in the non-relativistic approximation, to the well-known expression

\[ E_l = \frac{l(l + 1) \hbar^2}{2m^2}. \quad \text{(4)} \]

We next consider the more realistic case of a dumb-bell shaped rotator. It will be seen that the problem can be solved if we assume that the two particles of the rotator are of equal mass. The Hamiltonian for a pair of non-interacting particles of rest masses \( m_1 \) and \( m_2 \) is

\[ H = c \sqrt{m_1^2c^2 + \frac{p_1^2}{m_1}} + c \sqrt{m_2^2c^2 + \frac{p_2^2}{m_2}} \]

\[ = c \sqrt{m_1^2c^2 - \hbar^2 \nabla_1^2} + c \sqrt{m_2^2c^2 - \hbar^2 \nabla_2^2} \quad \text{(5)} \]

where we make the usual substitution \( \vec{p} = -i\hbar \nabla \) and \( \nabla_1 \) and \( \nabla_2 \) refer to the different particles. Just as in the non-relativistic case we transform to the relative co-ordinates

\[ x = x_1 - x_2; \ y = y_1 - y_2; \ z = z_1 - z_2 \]

and the co-ordinates of the centre of mass,

\[ X = \frac{m_1x_1 + m_2x_2}{m_1 + m_2}; \ Y = \frac{m_1y_1 + m_2y_2}{m_1 + m_2}; \ Z = \frac{m_1z_1 + m_2z_2}{m_1 + m_2}. \]

we then obtain

\[ \frac{\partial}{\partial x_1} = \frac{m_1}{M} \frac{\partial}{\partial X} + \frac{\partial}{\partial x}, \ \text{etc.}; \ M = m_1 + m_2 \]

\[ \frac{\partial}{\partial x_2} = \frac{m_2}{M} \frac{\partial}{\partial X} - \frac{\partial}{\partial x}, \ \text{etc.}; \]

\[ \frac{\partial^2}{\partial x_1^2} = \frac{m_1^2}{M^2} \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial x_1^2} + 2m_1 \frac{\partial}{M \partial X \partial x}, \ \text{etc.}; \]

\[ \frac{\partial^2}{\partial x_2^2} = \frac{m_2^2}{M^2} \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial x_2^2} - 2m_2 \frac{\partial}{M \partial X \partial x}, \ \text{etc.} \quad \text{(6)} \]
Since we are not interested in the translational motion of the system, we hold \( X, Y, Z \) constant and we obtain

\[
\nabla_1 = - \nabla_2 = \nabla = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)
\]

\[
\nabla_1^2 = \nabla_2^2 = \nabla^2.
\]

(6')

If now we take

\[
m_1 = m_2 = m; \quad mc^2 = \frac{\varepsilon}{2}
\]

(5) becomes

\[
H = \varepsilon \sqrt{1 - \frac{2\hbar^2 \nabla^2}{m\varepsilon}}.
\]

(7)

From the relativistic wave equation

\[(H - W) \psi = 0\]

we have on multiplying by \( H + W \) on the left

\[(H^2 - W^2) \psi = 0\]

and substituting from (7), we finally obtain

\[
\nabla^2 \psi + \left( \frac{W^2 - \varepsilon^2}{2\hbar^2 \varepsilon} \right) m \psi = 0
\]

(8)

which is the appropriate Klein-Gordon equation for our system.

With \( r = a; \ I = \mu a^2 \) where the reduced mass \( \mu = m/2 \) and \( \varepsilon = 2mc^2 \) the rest energy of the system, (8) goes over into (2) and we recover the formula (3) for \( W \).

We now proceed to determine the eigenvalues of \( W \) according to the Dirac equation. As before, we first consider the case of a single particle at a distance ' \( a \) ' from a centre of rotation. The Dirac equation

\[
c (a_x p_x + a_y p_y + a_z p_z + a_0 mc) \psi = W \psi; \quad a_i a_j + a_j a_i = 2\delta_{ij}
\]

(9)
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with the representation

\[ a_1 = \begin{pmatrix} \ldots & 1 \\ \\
. & 1 \\ \\
1 & . \\ \\
\end{pmatrix}, \quad a_2 = \begin{pmatrix} \ldots & -i \\ \\
. & i \\ \\
i & . \\ \\
\end{pmatrix}, \]

\[ a_3 = \begin{pmatrix} \ldots & 1 \\ \\
. & . & -1 \\ \\
1 & . & . \\ \\
\end{pmatrix}, \quad a_4 = \begin{pmatrix} \ldots & 1 \\ \\
. & . & -1 \\ \\
1 & . & . \\ \\
\end{pmatrix}. \]

leads to the set of differential equations (see, for example, Persico, Fundamentals of Quantum Mechanics, p. 430)

\[ \frac{i}{\hbar c} (mc^2 - W) \psi_1 + \left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \psi_4 + \frac{\partial}{\partial z} \psi_3 = 0 \]

\[ \frac{i}{\hbar c} (mc^2 - W) \psi_2 + \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \psi_3 - \frac{\partial}{\partial z} \psi_4 = 0 \]

\[ \frac{i}{\hbar c} (-mc^2 - W) \psi_3 + \left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \psi_2 + \frac{\partial}{\partial z} \psi_1 = 0 \]

\[ \frac{i}{\hbar c} (-mc^2 - W) \psi_4 + \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \psi_1 - \frac{\partial}{\partial z} \psi_2 = 0. \] (10)

In analogy with the solution of the hydrogen problem, but with \( r = a \), we attempt to solve the equations (10) by taking each of the four \( \psi_p (p = 1, 2, 3, 4) \) in the form

\[ \psi_p = a_p Z_l^m = a_p \sqrt{\frac{4\pi}{2l + 1}} (l + m)! (l - m)! \ Y_{lm}; \quad a_p \text{ const.} \]

where \( Y_{lm} \) is a surface harmonic. Taking \( r = a \), one can verify the following relations for \( Z_l^m \):

\[ \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) Z_l^m = - \frac{l}{(2l + 1) a} Z_{l+1}^{m+1} - \frac{(l - m) (l - m - 1) (l + 1)}{(2l + 1) a} Z_{l-1}^{m+1} \]
\[
\left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) Z_l^m
\]
\[
= \frac{l}{(2l + 1) a} Z_{l+1}^{m-1} + \frac{(l + m)(l + m - 1)(l + 1)}{(2l + 1) a} Z_{l-1}^{m-1}
\]
\[
\frac{\partial}{\partial z} Z_l^m
\]
\[
= - \frac{l}{(2l + 1) a} Z_{l+1}^m + \frac{(l + m)(l - m)(l + 1)}{(2l + 1) a} Z_{l-1}^m.
\] (11)

If now we take

\[
\psi_1 = ia_1 Z_{l+1}^m; \quad \psi_2 = ia_1 Z_{l+1}^{m+1}
\]
\[
\psi_3 = (l + m + 1) a_2 Z_l^m; \quad \psi_4 = -(l - m) a_2 Z_l^{m+1}; \quad a_1, a_2 \neq 0
\] (12)

substitution in (10) eliminates the spherical harmonics entirely; the first two of equations (10) yield

\[
W - mc^2 \frac{\hbar c}{\hbar c} a_1 - \frac{l}{a} a_2 = 0
\] (13)

and the second two equations yield

\[
\frac{l + 2}{a} a_1 - \frac{W + mc^2 \hbar c}{\hbar c} a_2 = 0.
\] (13')

In order that the system of equations (13) should have a non-trivial solution for \(a_1\) and \(a_2\), the determinant of the system should be zero, i.e.,

\[
W^2 - \varepsilon^2 = \frac{l(l + 2)}{a^2} \hbar c^2 = \frac{l(l + 2) \hbar c^2}{1}
\] (14)

or, we have for the eigenvalues of \(W\)

\[
W_l = \varepsilon \sqrt{1 + \frac{l(l + 2)}{1 \varepsilon}}; \quad l = 0, 1, 2, \ldots
\] (15)

On the other hand, taking

\[
\psi_1 = i (l + m) b_l Z_{l-1}^m; \quad \psi_2 = - i (l - m - 1) b_l Z_{l-1}^{m+1}
\]
\[
\psi_3 = b_2 Z_l^m; \quad \psi_4 = b_2 Z_l^{m+1}; \quad b_1, b_2 \neq 0
\] (16)

gives another solution of the equations (10) which results in
\[ W_l = \varepsilon \sqrt{1 + \frac{(l-1)(l+1)}{16} \hbar^2} \quad ; \quad l = 1, 2, 3, \ldots \quad (17) \]

which is the same as (15) with \( l - 1 \) written for \( l \).

Recalling the ideas of angular momentum in Dirac theory, we see that we can introduce the inner quantum number \( J \) defined by

\[ J = l + \frac{1}{2} \quad \text{for the solutions (12) and} \]

\[ = l - \frac{1}{2} \quad \text{for the solutions (16) and in terms of} \ J, \ (15) \quad \text{and} \ (17) \]

both can be written in the form

\[ W_J = \varepsilon \sqrt{1 + \frac{[J(J+1) - \frac{3}{4}] \hbar^2}{16}} \quad ; \quad J = \frac{1}{2}, \frac{3}{2}, \ldots \quad (18) \]

As is well known, the non-relativistic description of this situation is that the spin of the rotating particle is either parallel or antiparallel to the orbital angular momentum.

Before discussing the formula (15), we prove its validity as in the Klein-Gordon case for a system of two non-interacting particles of equal mass. One observes that taking the sum of two Dirac Hamiltonians as that of the system, leads in view of relations (6) to the uninteresting result that the total Hamiltonian refers merely to the centre of mass. We, therefore, start with the Klein-Gordon equation (8) in the form

\[ \left( \frac{W^2}{c^2} + 4\hbar^2 \nabla^2 - 4m^2c^2 \right) \psi = 0 \]

and seek the corresponding Dirac equation

\[ \left( \frac{W}{c} - \beta_1 p_x - \beta_2 p_y - \beta_3 p_z - \beta_4 mc \right) \psi = 0 \]

which is equivalent to (8). The operators \( \beta_i \) will obviously have to satisfy the commutation relations

\[ \beta_i \beta_j + \beta_j \beta_i = 8 \delta_{ij} \quad (20) \]

Hence \( \beta_i = 2a_i \) where \( a_i \) are the Dirac operators of (9). Taking \( W' = W/2 \) (19) becomes

\[ \left( \frac{W'}{c} - a_1 p_x - a_2 p_y - a_3 p_z - a_4 mc \right) \psi = 0 \]
which gives, as in the case of a single particle [cf. Equation (14)],

\[ W'^2 - m^2c^4 = \frac{l(l + 2)}{a^2} \hbar^2c^2. \]  

(21)

With

\[ W' = \frac{W}{2}; \varepsilon = 2mc^2; \quad l = \mu a^2 = \frac{m}{2}a^2 \]

we again arrive at (15) for the eigenvalues of the energy.

We now proceed to discuss the formulae (3) and (15). We have already seen that the formula (3) leads to the well-known wavemechanical formula (4) in the first order approximation. Carrying out the approximation a stage further, we have

\[ W_l = \varepsilon + l(l + 1) \hbar c B - \frac{l^2(l + 1)^2 \hbar^2c^2B^2}{2\varepsilon}, \]

(22)

where

\[ B = \frac{\hbar}{8\pi^2lc} \]

is the so-called "rotational constant" (see Herzberg, *Spectra of Diatomic Molecules*, p. 71). Introducing the wave number

\[ \nu_l = \frac{W_{l+1} - W_l}{\hbar c} \]

we obtain (in conformity with the selection rule \( \Delta l = \pm 1 \)), for the transition \( l + 1 \rightarrow l \)

\[ \nu_l = 2(l + 1)B - \frac{2\hbar cB^2}{\varepsilon} (l + 1)^2; \quad l = 0, 1, 2, \ldots \]

(23)

The second term of (23) is very much smaller than \( 4D(l + 1)^3 \) (see Herzberg) which would arise if one assumed that the rotator is non-rigid, and may not be detectable. However, in the empirical formula

\[ \nu = fm - gm^3, \]

we must therefore have

\[ f = 2B; \quad g = 4D + \frac{2\hbar cB^2}{\varepsilon}; \quad m = l + 1. \]  

(24)
The constant $g$ is extremely small in comparison with $f$ and neglecting the second term in (24) would lead to a spectrum consisting of nearly equidistant lines. Employing the more exact formula (23) for the "Rigid rotator" ($D = 0$) we obtain, for the line separation,

$$\nu_{l+1} - \nu_l = 2B - \frac{6hcB^2}{\varepsilon} [(l + 1)(l + 2) + \frac{1}{2}]; \ l = 0, 1, 2, \ldots$$

(25)

We next consider the formula (15) or equivalently (18) in terms of the quantum number $J = l + \frac{1}{2}$ which obviously takes into account the "spin" of the rotating particle. To the second order of approximation, (18) leads to

$$W_J = \varepsilon + [J(J + 1) - \frac{3}{4}] \hbar cB - \frac{[J(J + 1) - \frac{3}{4}]^2 \hbar^2 c^2 B^2}{2\varepsilon}$$

$$J = \frac{1}{2}, \frac{3}{2}, \ldots$$

(26)

from which we have

$$\nu_J = 2(J + 1)B - \frac{\hbar c B^2}{2\varepsilon} (J + 1)(4J^2 + 8J + 1); \ J = \frac{1}{2}, \frac{3}{2}, \ldots$$

(27)

Neglecting the second term, for the moment, we immediately find that the first rotational line $\nu$ lies at $3B$ and not at $2B$ which is the case according to the non-relativistic or even the Klein-Gordon equation. This circumstance would show whether the atoms of a homonuclear diatomic molecule should be considered as Dirac particles or Klein-Gordon particles. To this order of approximation the line separation is $2B$ in this case also. On the other hand the formula analogous to (25) is

$$\nu_{J+1} - \nu_J = 2B - \frac{6hcB^2}{\varepsilon} \left[(J + 1)(J + 2) + \frac{1}{12}\right]; \ J = \frac{1}{2}, \frac{3}{2}, \ldots$$

(28)

We wish to express our gratitude to the Council of Scientific and Industrial Research for the award of a Fellowship to one of us (D. S.) and to Dr. Syed Ziauddin for kind interest.

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