

Relativistic Quantum Mechanics of the Hydrogen Atom as the Weak-Field Limit of a Nonlinear Theory

ANTONIO F. RAÑADA

Departamento de Física Teórica and GIFT, Universidad Complutense, Madrid-3, Spain

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Abstract

The effect of nonlinear terms in the Dirac equation is investigated, in the case of the hydrogen atom. It is found that the change in the energy is of order α^6 for a very large range of values of the coupling constant of the dominant term. It is shown that a nonlinear classical field theory has a quantumlike behavior near the linear limit. This implies the existence of a close relation between linearization and quantization. A classical stable model of the hydrogen atom is presented. Some consequences are discussed.

1. Introduction

We could define elementary physics as the physics of linear phenomena. The pendulum, an elastic rod, any optical system, etc., are first studied as linear systems, described by linear differential equations. But when more precision is necessary, the effect of nonlinear terms in the equations must be considered. This usually happens when the physical magnitudes of the problem turn out to be very big or when the experimental errors are very small..

This transition from a linear, approximate theory to a nonlinear, more exact one is general in physics. There is, however, a very important exception to this rule: quantum mechanics. The reason is, of course, that physicists are used to thinking that in order to go beyond quantum mechanics it is better to construct a completely new formalism, the second quantization. No doubt, quantum field theory makes use of nonlinear equations. But in general the nonlinearity is due to the interactions and, at least in the simplest theories, does not appear in the case of free particles.

It is surprising that no more attention has been paid to the development of a nonlinear quantum mechanics without second quantization. In such a theory the classical solution of the field equations—and, in fact, the classical theory of fields—would play a very important role concerning the transit from quantum mechanics to elementary particle physics. It is usually assumed that the typical discontinuous phenomena of the atomic world are inaccessible to

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a classical theory. However, the oldest known quantum phenomena, such as the quantization of energy, have a classical analogy in the case of the frequencies of vibration and they appear in nonlinear classical field theory. On the other hand, the very rich and almost unknown world of the stability of the solutions of nonlinear partial differential equations offers a very suggestive formalism for the study of quantum jumps. It is evident that this point of view does not have much chance of being easily accepted among high-energy physicists. Nevertheless, its degree of credibility should have increased considerably after one of the most fascinating discoveries in many years of mathematical physics: the soliton.

As is well known, a soliton is a localized, traveling wave that preserves its shape upon collision with other analogous waves. For a general review we refer to Whitham (1974) and Scott et al. (1973), where its applications to many branches of physics are studied, together with a description of the empirical discovery of the soliton in 1831. Of course, solitons only appear in nonlinear equations. Given a localized, traveling wave (also called solitary wave or kink) it is difficult to know if it is a soliton, that is, if it is able to reconstruct itself after collisions. In one dimension the problem can be solved in some cases by means of the inverse scattering method (Whitham, 1974; Gardner et al., 1967). However, in three dimensions the problem is very difficult in spite of some important recent results (Zakharov and Kuznetsov, 1974).

The great stability of the soliton makes it an ideal tool for representing elementary particles. The preservation of shape after collisions could be used to explain elastic scattering, while in inelastic processes the interaction terms, acting as sources, would produce new solitons.

We may quote some interesting proposals in this connection, such as those of Skyrme (1961a,b) and Caudrey et al. (1975), which are not, however, realistic because they use one-dimensional fields. On the other hand, there are more realistic three-dimensional models with scalar (Anderson and Derrick, 1970) and Dirac fields (Finkelstein et al., 1951, 1956; Soler, 1970, 1973; Rañada and Soler, 1973) It has even been possible to construct classical models of nucleons, as the kinks or solitary waves of nonlinear Dirac fields (Rañada et al., 1974) or of a system of nonlinear Dirac and pseudoscalar fields in interaction (Rañada and Vazquez, 1976). However, it is not known if the solutions that these models use are solitons or merely solitary waves, although they are stable, as has been shown by Soler (1975).

A great effort is presently being made in the quantization of nonlinear field theories (Coleman, 1975; Christ and Lee, 1975). Although this line of work causes at this moment great excitement, we take a different approach and concentrate on the effect of nonlinear terms at the classical level, that is, without second quantization.

On the other hand, there are very powerful dynamical reasons that demand the existence of nonlinear terms in the field equations. Weyl (1950) showed that if the gravitation is introduced in the so-called "mixed" way, by considering the metric and the affine connection as independent quantities, the spinor fields must obey either linear equations in a space with torsion or nonlinear

equations in a Riemann space. The application of Weyl's idea to a simple model of the universe leads precisely to the nonlinear Soler model (Soler, 1970a; Rañada and Soler, 1972).

All these considerations point to the necessity of somehow including nonlinear terms in the free field equations. These terms should appear some way at the level of quantum mechanics. But quantum mechanics is a linear theory that has reached a tremendous success in the prediction of experimental data in the physics of the so-called quantum world. A very interesting problem arises: Is it possible to introduce nonlinearities without spoiling the very beautiful features of quantum mechanics?

A first hint to the answer might be found in the fact that quantum mechanics describes the particles better, when the extension of the wave function is much bigger than the Compton wavelength (e.g., the hydrogen atom) than when the situation is the opposite one (e.g., the free electron). It is clear that in the first case the field must be weak and the linear approximation can be adequate, while we cannot expect the same thing in the second one. Moreover, if the potential is very strong, as in the case of the Coulomb field of a nucleus, its effect must dominate over that of the nonlinear terms, which on the other hand would be dominant in a free particle (Soler, 1970b). Another argument that should be considered is that only a nonlinear theory can avoid the annoying broadening of any wave packet. It is therefore convenient to study the possibility of a nonlinear quantum mechanics.

In the present work, we study in a quantitative way all these qualitative considerations, in the case of the Dirac equation in the hydrogen atom. More precisely, we take the following nontrivial problems: Is relativistic quantum mechanics of the hydrogen atom the linear limit of a nonlinear theory? Is it possible to detect experimentally the hypothetical nonlinear terms? As we will see the answer is that for a very broad range of values of λ , the coefficient of the dominant term $(\psi\psi)^2$, the nonlinear effects are of order α^6 and cannot be detected experimentally.

In Section 2 we study the linearization of a general nonlinear theory in the hydrogen atom. We show that the introduction of an action constant is a necessary condition to linearize properly a classical field theory. The equations of the first nonlinear approximation are solved numerically and the results are explained in Section 3. In Section 4 we interpret and comment on these results. In Section 5 we propose a classical nonlinear model of the atom, and finally in Section 6 we summarize the problem and state the conclusions.

2. The Linearization Problem

We take the following problem: Is it possible to represent the electron in a hydrogen atom by a nonlinear Dirac field, in such a way that the theory coincides with quantum mechanics, at least within the limits of experimental errors? To be precise the last sentence will be understood to mean up to α^4 order, α being the fine-structure constant.

At first thought, the problem may seem to be trivial, the answer being

affirmative. In fact, in the hydrogen atom the electron is very extended and its field must be very weak. Moreover, the Coulomb potential is very intense near the nucleus, where the nonlinear terms are expected to be more important. This seems to suggest that the potential must dominate over the self-coupling and that the linear approximation may be adequate. The problem is not, however, as simple as that. The preceding arguments do not consider two very important aspects of the question: The norm of the solutions and the determination of the frequency and the energy.

In quantum mechanics the norm of a solution is not determined by the equation but the wave function is normalized to unity once it is obtained. In a nonlinear theory there is no such freedom because the norm is imposed by the equation. As a consequence a nonlinear theory can linearize to quantum mechanics only if for all the sets of quantum numbers (n, j, l, m) there exist solutions such that

$$\|\psi_{nljm}\| = \int |\psi_{nljm}|^2 d^3r \quad (2.1)$$

has the same value, independently of (n, j, l, m) . Of course, one cannot know a priori if this is the case.

The frequency is fixed in quantum mechanics by the requirement that the wave function be well behaved both at the origin and at infinity (Akhiezer and Berestetskii, 1965). However, the same argument does not apply in nonlinear theory because the square integrable solutions behave as the linear wave functions for $r \rightarrow \infty$ but not for $r \rightarrow 0$. The method used in quantum mechanics to determine ω is not, therefore, valid in nonlinear theory. Let us take a second look into these two problems.

We consider the class of nonlinear equations with the Dirac equation as linear part and with a nonlinear part that can be developed in a series of bilinear covariants. Being interested in the weak-field limit, we keep only up to fourth order in the Lagrangian; that is, we take

$$L = L_L + L_{NL} \quad (2.2)$$

where

$$L_L = \frac{1}{2}(\bar{\psi}\gamma^\mu\partial_\mu\psi - (\partial_\mu\bar{\psi})\gamma^\mu\psi) - m\bar{\psi}\psi - e\bar{\psi}\gamma^0\psi A_0 \quad (2.3)$$

A_0 is the electrostatic potential of the nucleus and L_{NL} is the most general combination of fourth order, that is, constructed with the bilinears S, V, T, A, P (Finkelstein et al., 1956).

$$L_{NL} = \sum_{\sigma=1}^5 C_\sigma(\bar{\psi}\bar{\Gamma}_\rho^{(\sigma)}\psi)(\bar{\psi}\Gamma_\rho^{(\sigma)}\psi) \quad (2.4)$$

where $\Gamma_\rho^{(\sigma)}$ are the matrices of the Clifford algebra generated by $\{\gamma^\mu\}$. The four spinors in (2.4) being the same, one has

$$\begin{aligned} S + T - P &= 0 \\ V - A &= 0 \\ S - A + P &= 0 \end{aligned} \quad (2.5)$$

and L_{NL} can be written in the form

$$L_{NL} = \lambda [(\bar{\psi}\psi)^2 + b(\bar{\psi}\gamma^5\psi)^2] \tag{2.6}$$

This means that the most general fourth-order self-interaction is a combination of scalar $(\bar{\psi}\psi)^2$ and pseudoscalar $(\bar{\psi}\gamma^5\psi)^2$ couplings.

In order to solve classically the field equations, we must factorize the solutions in spherical coordinates. This is only possible if $b = 0$ and $j = 1/2$ simultaneously. When this is not the case we have to make a multipole expansion and write down equations for each partial wave. It is, however, much simpler to substitute a multipole approximation in the Lagrangian, integrate over the angles, and make variations of the radial functions. This procedure gives a low-order variational approximation to a solution. We will take spinors of the form

$$\psi_{jlj_s}(\mathbf{r}) = e^{-i\omega t} \begin{pmatrix} g(r)\mathscr{Y}_{j_l}^{j_s} \\ if(r)\mathscr{Y}_{j_l}^{j_s} \end{pmatrix} \tag{2.7}$$

where $\mathscr{Y}_{j_l}^{j_s}$ are the spinor spherical harmonics and l' depends on l, j in the usual way.

Substitution of (2.7) in (2.2) and integration over the angles results in

$$\begin{aligned} L_L &= \int_0^\infty \left[gf' - fg' - 2\kappa \frac{gf}{r} + (\omega - eA_0)(g^2 + f^2) - m(g^2 - f^2) \right] r^2 dr \\ L_{NL} &= \lambda \int_0^\infty \left[C_1(k)(g^2 - f^2)^2 - 4bC_2(k)g^2f^2 \right] r^2 dr \end{aligned} \tag{2.8}$$

where κ is the eigenvalue of $\beta \cdot (\bar{\Sigma} \cdot \bar{L} + 1)$ and

$$C_1(k) = \int |Y_{|\kappa|-1}^{|\kappa|-1}|^4 d\Omega, \quad C_2(k) = \int |Y_{|\kappa|-1}^{|\kappa|-1}|^4 \cos^2\theta d\Omega \tag{2.9}$$

It is convenient to make the following change of variables and parameters:

$$\begin{aligned} (g, f) &= \left[\frac{m}{2|\lambda|C_1(k)} \right]^{1/2} (G, F), \quad A_0 = \frac{m}{e} V \\ \rho &= mr, \quad \Lambda = \omega/m \end{aligned} \tag{2.10}$$

which leads to

$$\begin{aligned} L &= \frac{1}{2|\lambda|m^2C_1(k)} \\ &\times \left\{ \int_0^\infty \left[GF' - FG' - 2\kappa \frac{GF}{\rho} + (\Lambda - V)(G^2 + F^2) - (G^2 - F^2) \right] \rho^2 d\rho \right. \\ &\left. + \frac{1}{2} \text{sg}\lambda \int_0^\infty (G^2 - F^2)^2 \rho^2 d\rho - 2b \text{sg}\lambda \frac{C_1}{C_2} \int G^2 F^2 \rho^2 d\rho \right\} \end{aligned} \tag{2.11}$$

As we see, $|\lambda|$ and m are scale parameters. Being near the linear limit, G and F turn out to be large and small components as in linear quantum mechanics. For this reason the pseudoscalar term is negligible as compared with the scalar one, if b is of the order of unity. For instance the difference in the energy between $b = 0$ and $b = -1$ (corresponding to scalar and pseudovectorial self-couplings) is only of order α^8 . From now on we will take $b = 0$. In other words the linear limit is dominated by the $(\bar{\psi}\psi)^2$ term.

In (2.11) we vary the radial functions and obtain

$$\begin{aligned} F' + \frac{(1-\kappa)}{\rho} F - (1-\Lambda+V)G - \text{sg}\lambda(F^2 - G^2)G &= 0 \\ G'_\psi + \frac{(1+\kappa)}{\rho} G - (1+\Lambda-V)F - \text{sg}\lambda(F^2 - G^2)F &= 0 \end{aligned} \quad (2.12)$$

These equations are exact if $|\kappa| = 1$, that is in $S_{1/2}$ and $P_{1/2}$ waves. In the other cases they must be understood as lowest wave approximations. If we take for $V(\rho)$ a purely Coulomb field there are no square integrable solutions if $j = 1/2$. The reason is that the nonlinear term amplifies the singularity that the $j = 1/2$ wave functions have at $\rho = 0$. This problem does not arise if $j > 1/2$. Fortunately the electrostatic potential is not purely Coulombic because of the finite size of the proton. We have taken

$$v(\rho) = \begin{cases} -\frac{\alpha}{\rho}, & \rho > R_0 \\ -\frac{\alpha}{R_0} \left(\frac{3}{2} - \frac{1}{2} \left(\frac{\rho}{R_0} \right)^2 \right), & \rho \leq R_0 \end{cases} \quad (2.13)$$

which is the potential produced by a sphere of radius R_0 with uniform charge density. The mean square radius is $\langle \rho^2 \rangle^{1/2} = (3/5)^{1/2} R_0$.

The energy comes out from the energy momentum tensor

$$T^{\alpha\beta} = \frac{i}{2} [\bar{\psi}\gamma^\alpha \partial^\beta \psi - (\partial^\beta \bar{\psi})\gamma^\alpha \psi] + g^{\alpha\beta} \lambda (\bar{\psi}\psi)^2 \quad (2.14)$$

where we have used the equation

$$L = -\lambda (\bar{\psi}\psi)^2 \quad (2.15)$$

which is valid for the solutions of the field equations. The effect of the interaction does not appear explicitly but is included in (2.14) and (2.15). One has

$$E = \int T^{00} d^3r = \omega \int \psi^+ \psi d^3r + \lambda \int (\bar{\psi}\psi)^2 d^3r \quad (2.16)$$

where the linear and nonlinear components of the energy appear clearly separated.

The norm of the solutions is

$$N = \|\psi\| = \int \psi^+ \psi d^3r \quad (2.17)$$

In linear theory it is usually stated that N is set equal to unity by means of a normalization factor. This is not completely correct because N has dimensions

of action. To normalize to unity is in fact to normalize to the Planck constant \hbar . In a nonlinear theory N is a function of λ and m . More precisely, (2.16) and (2.17) can be written (we take $j = 1/2$, for which $C_1 = 1/4\pi$) as

$$E = \frac{2\pi}{|\lambda|m} (\Lambda I_1 + \frac{1}{2} \operatorname{sg}\lambda I_2) \tag{2.16'}$$

$$N = \frac{2\pi}{|\lambda|m^2} I_1 \tag{2.17'}$$

where

$$I_1 = \int_0^\infty (G^2 + F^2) \rho^2 d\rho \tag{2.18}$$

$$I_2 = \int_0^\infty (G^2 - F^2)^2 \rho^2 d\rho$$

I_1 and I_2 depend on Λ but not on $|\lambda|$ or m . It turns out that F, G are very small so that $I_2 \ll I_1$. For instance in the ground state we will find that $I_2/I_1 < 10^{-11}$ in the case of the relevant solutions.

From (2.16') and (2.17') it follows then

$$E = \Lambda m N = N \omega \tag{2.19}$$

As we have explained before, a necessary condition for a theory to linearize to quantum mechanics is that the norm of the different states be the same. In that case (2.19) shows that N plays the role of quantum of action and must be equal to \hbar , the Planck constant. In nonlinear field theory the Planck constant can thus be interpreted as the norm of the electron field. If we take the linear approximation we can no longer calculate the value of this norm, and it must be introduced as a fundamental constant in order to overcome the insufficiency of the theory. A close relation appears thus between quantization and linearization: From the point of view of nonlinear classical field theory, an action constant must be introduced in order to assure the correctness of the linearization. In other words, quantization is a necessary condition to linearization. As we will see, the fact that N has to take the same value for all the different states does not present any problem.

Let us now consider the second problem: the determination of $\Lambda = \omega/m$. In linear theory the solutions are of the form

$$\begin{aligned} r g &= (1 + \Lambda)^{1/2} e^{-\sigma r} (F_1 + F_2) \\ r f &= (1 - \Lambda)^{1/2} e^{-\sigma r} (F_1 - F_2) \\ \sigma &= (m^2 - \omega^2)^{1/2} \end{aligned} \tag{2.20}$$

where

$$\begin{aligned} F_1 &= c \frac{\gamma - \alpha\omega/\sigma}{-\kappa + \alpha m/\sigma} z^\gamma M(\gamma + 1 - \alpha\omega/\sigma; 2\gamma + 1; z) \\ F_2 &= c z^\gamma M(\gamma - \alpha\omega/\sigma; 2\gamma + 1; z) \end{aligned} \tag{2.21}$$

where c is a constant, $\gamma = (\kappa^2 - \alpha^2)^{1/2}$, $z = 2\sigma r$, and M is the Kummer function. In order that F_1 and F_2 do not blow up at infinity, Λ must take some precise values. This argument does not apply in nonlinear theory because we only need solution of the linear equation well behaved at infinity. The reason is that near the origin the linear and nonlinear solutions do not have the same behavior. In fact for any Λ we have the asymptotic solution

$$F_1 = cz^\gamma \frac{(\gamma - \alpha\omega/\sigma)(-\gamma - \alpha\omega/\sigma)}{-\kappa + m\alpha/\sigma} U(\gamma + 1 - \alpha\omega/\sigma; 2\gamma + 1; z)$$

$$F_2 = cz^\gamma U(\gamma - \alpha\omega/\sigma; 2\gamma + 1; z)$$
(2.22)

where $U(a; b; z)$ is defined as (Abramowitz and Stegun, 1972)

$$U(a; b; z) = \frac{\pi}{\sin\pi b} \left[\frac{M(a; b; z)}{\Gamma(1 + a - b)\Gamma(b)} - z^{1-b} \frac{M(1 + a - b; 2 - b; z)}{\Gamma(a)\Gamma(2 - b)} \right]$$
(2.23)

When $\Lambda = \omega/m$ takes any of the values that the linear theory predicts, (2.22) and (2.21) are proportional. U is divergent at $\rho = 0$ but is well behaved at infinity:

$$U(a; b; z) = z^{-a} [1 + O(|z|^{-1})]$$

$$|z| \rightarrow \infty$$

We cannot thus exclude any value of Λ . In fact we have found a continuous family of solutions. The frequency seems thus undetermined.

In order to understand our problem more clearly, let us consider a process that presents a close analogy with it: the buckling of a rod submitted to axial stress (Reiss, 1969). Let the rod be placed along the x axis with its ends at $x = 0$ and $x = 1$. Under axial stress, the endpoints suffer a displacement c . According to the linear theory of elasticity, the rod buckles only if c takes one of the critical values $c_n = \beta(n\pi)^2/2$, β being a physical constant. In that case the shape of the rod is given by

$$w_n(x) = A_n \sin n\pi x$$

with an undetermined amplitude A_n . When nonlinear terms are introduced, it turns out that c is not restricted to the critical values but the rod can buckle into the shape $\sin n\pi x$ if $c \geq c_n$, the amplitude being given by

$$c = c_n(1 + A_n^2/4\beta)$$

The situation is analogous in our case. The linear theory fixes ω but not the norm, while the nonlinear theory allows a continuum of values of ω but determines the norm as a function of ω . By the way, the preceding example presents the existence of an infinity of unstable classical states with increasing energies: the buckled states with $n = 1, 2, 3 \dots n \dots$. The rod can make classical transitions to the state of minimum energy, with an evident quantum aspect.

To sum up we need to know the following:

(i) Are the nonlinear solutions also approximate linear solutions, and, if so, with what degree of approximation?

(ii) Which are the allowed frequencies in a nonlinear theory?

(iii) Which are the norms of the nonlinear solutions? More precisely: is there a complete set of solutions, all of which have the same norm?

We have not been able to answer these questions analytically. We have thus solved the problems by performing a numerical analysis of the equations.

3. Numerical Results

We have solved equation (2.12) with the potential given by (2.13) in the waves $1S_{1/2}; 2S_{1/2}; 2P_{1/2}; 3S_{1/2}; 3P_{1/2}$. The reason for limiting our work to the case $j = 1/2$ is that, if $j = 1/2$, (2.12) being only the lowest wave approximation, several multipoles must be considered, making the calculation much longer. Nonetheless the pattern of our results seems to be general. In order to solve the equation we have proceeded as follows.

First of all we fixed the values of the parameters Λ and R_0 . In the case of S waves the function F must vanish at $\rho = 0$ and the only initial condition is $G(0)$. It turns out that there are two kinds of solutions: If $G(0)$ is bigger than a certain value G_0 , the behavior when $\rho \rightarrow \infty$ is $G \rightarrow -\infty, F \rightarrow +\infty$, while if $G(0) < G_0$ it is $G \rightarrow +\infty, F \rightarrow -\infty$. This value can be considered as corresponding to a square integrable solution. Of course, it cannot be determined exactly, but we can approach it as much as we want. The more we approach it, the farther the tendency of G, F to diverge appears. In practice it is better to calculate $G/G_l; F/F_l$, where G_l, F_l are well-known linear solutions, normalized such that

$$\int_0^\infty (G_l^2 + F_l^2) \rho^2 d\rho = 1$$

That calculation shows that $G/G_l, F/F_l$ approach the same constant C , over an increasing interval when $G(0) \rightarrow G_0$. For instance when G_0 is determined with three significant figures these quotients are constant up to six figures from below $r = 0.004 \text{ \AA}$, to over $r = 8 \text{ \AA}$, and this result can be improved very easily. In other words, the nonlinear solutions are very approximately proportional to the linear ones. Of course, we should keep in mind that when ω does not take a linear value G and G_l correspond to different frequencies. The preceding statement applies when the difference between ω and a linear value ω_l is not big (smaller than $10^3 \alpha^6$, for instance). However, we will be mainly interested in such cases and therefore the quotients G/G_l and F/F_l are very useful in the numerical process.

For P waves the only difference is that $G(0) = 0$ and we have to determine $F(0)$. The method is very similar to the one used by Finkelstein et al. (1951) and Soler (1970a), and it appears plotted in Figure 1.

Concerning the value of the parameters R_0 and Λ we proceeded as follows. R_0 measures the size of the nucleus. We have studied the interval between

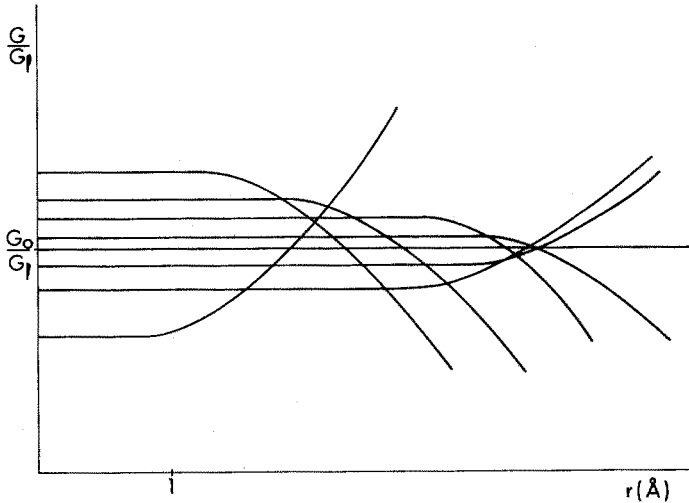


Figure 1. G/G_1 versus r for several solutions in the $1S_{1/2}$ wave.

$R_0 = 0.0022$ and $R_0 = 0.0032$ which correspond to $\langle r^2 \rangle_p^{1/2} = 0.65$ fermi and $\langle r^2 \rangle_p^{1/2} = 0.95$ fermi, $\langle r^2 \rangle_p^{1/2}$ being the mean square charge radius of the proton. The experimental value falls inside this interval, and in this way we have determined the sensitivity of our results to small variations of R_0 . As we showed before, there are no special values for Λ . The calculation proves that there is a family of solutions corresponding to a continuum of Λ . It is convenient to write

$$\Lambda = \Lambda_l + \frac{2\pi e^2}{5} R_0^2 |\varphi(0)|^2 + A\alpha^6 \quad (3.1)$$

The first term is the linear eigenvalue for a Coulomb field as given by the fine-structure formula. The second one is the correction due to the finite size of the nucleus, calculated in lowest-order perturbation theory, φ being the Schrödinger wave function. It is of order $\alpha^4(mR_0)^2$ or equivalently of α^6 order. The third term measures the difference between the linear and the nonlinear eigenvalues. We take this form because our computer does not appreciate the α^8 terms. According to the theory of nonlinear partial differential equations the nonlinear solutions must bifurcate from the zero solution at a linear eigenvalue, that is at $A = 0$, in complete agreement with our results.

For every couple of values of R and A we have found one of $C = G/G_1 = F/F_l$. The results show that (i) there are no square integrable solutions if $\text{sg}A = \text{sg}\lambda$; (ii) when $\text{sg}A = -\text{sg}\lambda$ there is a solution for any value of A , at least in the interval $10^{-4} < |A| < 10^{10}$. The relation $C = \text{const.} \times |A|^{1/2}$ holds at least with four significant figures; (iii) when $A \rightarrow -A$ and $\lambda \rightarrow -\lambda$, C does not change at least in the first four significant figures.

The results are plotted in Figure 2. Owing to the $C - A$ relation, quoted

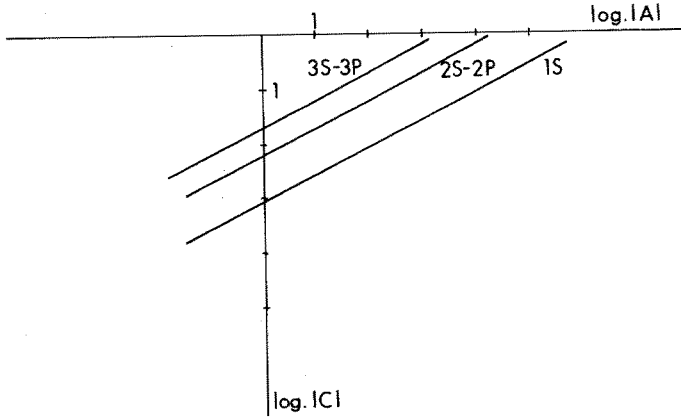


Figure 2. Log $|C|$ versus $\log |A|$ for the waves with $n = 1, 2, 3$ and $j = 1/2$. Curves corresponding to the same n and j coincide.

above, $\log |C|$ is a linear function of $\log |A|$. The results do not depend on R , which appears in the problem only through the second term of (3.1). It is clear that when $A \rightarrow 0$, or equivalently, the nonlinear eigenvalue tends to the linear one, the nonlinear solution tends to zero. In other words the linear eigenvalue is a bifurcation point.

Now we turn to the energy and the norm. Because of the normalization of $G_l, F_l, I_1 = C^2$. We have thus, from (2.16') and (2.17'),

$$|\lambda| mE = 2\pi(\Lambda C^2 + \frac{1}{2} \text{sg} \lambda I_2) \tag{3.2}$$

$$|\lambda| m^2 N = 2\pi C^2 \tag{3.3}$$

Since C is function of A , (3.2) and (3.3) state that the energy and the norm depend on A . That is

$$E = E(A) = E(\Lambda) \quad N = N(A) = N(\Lambda)$$

We have stated that $I_2 \ll I_1$. This is clearly understood from the preceding results and from Figure 2. For instance, in the 1S wave if $|A| = 0.1$ one has $I_2/I_1 \sim 10^{-14}$ and if $|A| = 100$ $I_2/I_1 \sim 1.2 \times 10^{-11}$.

After equation (2.11) we have taken $b = 0$ because we expected the effect of the pseudoscalar term to be negligible. In order to test this approximation, we have repeated some of the calculations with $b = -1$, which corresponds to a pseudovector self-interaction. In fact, this is the type of self-coupling that follows directly from Weyl's idea (Weyl, 1950). The change affects C in the fifth significant figure. This means that the energy is affected on the order of α^8 .

4. Interpretation of the Results

In each of the five waves that we have considered, we found a family of solutions depending continuously on $\Lambda = \omega/m$. In the work of Soler (1970a,

1973) the situation is analogous and the arbitrariness of the frequency is solved by a principle of minimum energy, which states that the physical frequencies correspond to minima of the curve $E = E(\Lambda)$. However, in our case these curves have no minimum, as one can see very easily from (3.2) and Figure 2. In fact, the energy is very closely proportional to C^2 , which decreases to zero when $|A| \rightarrow 0$. Nonetheless, this does not imply that the energy is not fixed by the theory. In order to understand better the problem, let us consider the process of formation of a hydrogen atom. A free electron is bound by a proton in a state labeled by the quantum numbers (n, j, l, j_z) . If the initial value of Λ does not correspond to a minimum of $E(\Lambda)$ it will try to radiate energy until a minimum is reached. But, as we know, there are no minima in our case. We could be tempted to deduce that the energy must decrease until $C \rightarrow 0$, when $|A| \rightarrow 0$ and that the fields F, G , must vanish in this limit. The process would be very similar to the shrinking of the classical atom with a point electron. However, this process would violate the conservation of the norm N or the charge $q = eN$. If we restrict ourselves to stationary solutions, when the atom is formed the value of Λ must take a value such that the norm of the solution is equal to the norm of the free electron, which plays the role of an action constant. The energy will thus be well defined and will be

$$E = N\omega$$

even if $E(\Lambda)$ has no minimum. Of course in this formula we have neglected the unobservable effect of I_2 .

This suggests an interesting possibility: the determination of the action quantum as a nonfundamental constant, through the classical solution of the free-electron equations. It would be equal to the norm of the kinks or solitons representing the free electron in a nonlinear theory. Of course the value of this norm would play the role of action constant only in the case of the hydrogen atom, or perhaps, in the more general case of the Dirac field. We do not claim that this work implies that it is a universal constant, as happens in quantum mechanics. From the point of view of classical nonlinear theory the problem is as interesting as difficult.

From (3.3) we deduce (in natural units from now on)

$$C^2 = \frac{|\lambda|m^2}{2\pi} \quad (4.1)$$

Since C is function of $|A|$, (4.1) establishes a function

$$|A| = F(|\lambda|m^2)$$

which appears plotted in Figure 3. Given a value of λ , A is determined and, therefore, also Λ and E . In Figure 3 we use $\log |A|$ and $\log(|\lambda|m^2)$ because there is a simple relation between these quantities.

The curves corresponding to $+\lambda$ and $-\lambda$ are very close, the difference being too small to appear in the drawing. As we see if $|\lambda|m^2 < 10^{-4}$ $\Lambda - \Lambda_l < 10\alpha^6$ in all the waves. As the experimentally significant part of the fine

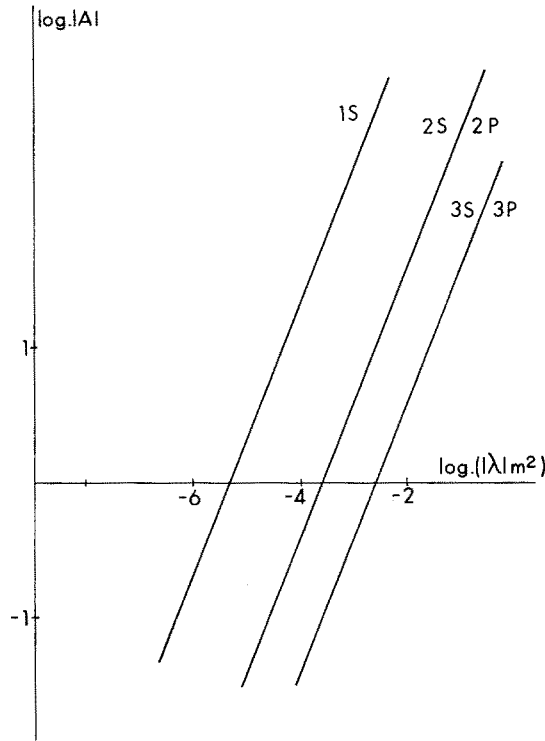


Figure 3. $\log |A|$ versus $\log (|\lambda| m^2)$ for the waves with $n = 1, 2, 3$, and $j = 1/2$. Curves corresponding to the same n and j coincide.

structure formula contains only up to α^4 terms, the differences in energy introduced by the self-coupling are not observable. For comparison, let us recall that the Fermi constant G is $Gm^2 \sim 10^{-11}$. We can also point out that two models of the nucleon have been proposed, considering nonlinear Dirac fields with $|\lambda| m^2 \sim 10^{-7}$ (Rañada et al., 1974; Rañada and Vazquez, 1976). Then a model of the electron with the same self-coupling constant is conceivable.

A final comment is due concerning the precision of our numerical calculations. The values of $G(0)$, C , the integrals, etc., are calculated with errors smaller than 0.1%. This is enough because a reduction of the error would only amount to a variation of less than 0.1% in the nonobservable value of A .

5. Classical Model of the Hydrogen Atom

The preceding results can be used to construct a classical model of the hydrogen atom. In it each state is given by a solution of a nonlinear field equation. We have only calculated five waves, but it seems reasonable to expect

that the pattern of results can be extended to all the spectrum. Given a value of λ , in a very large interval, the nonlinear and linear solutions differ very little, in α^6 order, when the latter are normalized to \hbar . The energy differences between both theories are smaller than the experimental errors.

Several kinds of objections can be presented to this model, for instance the following.

(i) This model is very similar to quantum mechanics. In fact, in the hydrogen atom the choice between linear and nonlinear theory is just a question of personal taste. The linear theory is much simpler and, therefore, much better.

(ii) Contrary to classical models, based on point electrons, this one is too stable because the electromagnetic current

$$j^\mu = e\bar{\psi}\gamma^\mu\psi$$

is time independent. No spontaneous radiation is predicted, in clear disagreement with experiments.

(iii) This model implies that the free electron must be an extended particle because it would be represented by the kinks or solitons of nonlinear Dirac and electromagnetic fields in interaction. However, it is usually stated that the electron has no structure.

(iv) A classical theory of the Dirac field cannot account for the Pauli exclusion principle.

Concerning the first objection, it must be stressed that the nonlinear classical theory can be reduced to a linear theory plus an action constant only in certain cases, as in the hydrogen atom. In these cases the linear theory is much simpler and the nonlinear one has no advantage. However, for free particles the predictions of linear and nonlinear theories are completely different. For instance, if we take the free solutions of the theory given by the Lagrangian (2.8) (with $A_0 = 0$) we obtain the Soler model, in which the particle has dimensions of order $1/m \approx 400f = 4 \times 10^{-3}$ Å. However, the linear theory has no stable, localized solitary waves. Of course, if the particle is very localized, it is necessary to take into account its own electromagnetic field which can play a fundamental role. Another important difference arises in the study of transitions. This brings about the second objection. First, let us remark that quantum mechanics predicts, in its simplest form, that the states are completely stable. In order to study the problem more deeply, we must consider the theory of stability of solutions of nonlinear, partial differential equations. If our solutions are not stable, the small perturbations produced by neighboring atoms, background radiation, etc., could induce transitions. If this is the case, an isolated atom would be stable, while one that is near matter would not. The problem is very difficult because the theory of stability in the case of partial differential equations is just beginning to develop. An interesting approach to the problem is proposed by Anderson and Derrick (1970) and Anderson (1971) in the case of the nonlinear scalar field. The transitions would be analogous to those that occur between buckled states of a rod (Reiss, 1969) or between different states of an anharmonic oscillator (Landau and Lifshitz, 1958). We cannot state that quantum transitions follow such a mechanism. However, the

present knowledge of the stability of partial differential equations does not seem sufficient to exclude this possibility.

Let us now take the third objection. The statement that the electron has no structure must be understood as meaning that its size is too small to be appreciated in present-day experiments. It is necessary to know if there are very localized solitons in the interaction of nonlinear Dirac and electromagnetic fields. The limit situation in which the spinor self-coupling is completely dominated by the electromagnetic coupling corresponds to the case studied by Wakano (1966), who found that there are no solitary waves. The opposite situation, in which the electromagnetic interaction is small and can be treated as a perturbation of the self-coupling, was studied by Soler (1973), Rañada and Soler (1973), Rañada et al. (1974), and Rañada and Vazquez (1976). The existence of solitary waves was proved, which were shown to be adequate to represent nucleons but not electrons. The intermediate case, in which both effects are comparable, is not known. We are presently working on this interesting problem. If these hypothetical, very localized spinorial, solitons do exist a classical model of the electron could be attempted. The predictions of this model concerning the hydrogen atom would be equal to those of quantum mechanics, up to α^4 order. Nevertheless, the interpretation of the field ψ would be different from that of the orthodox Copenhagen point of view. The electron would be an extended particle, whose size could change drastically, according to the different conditions to which it can be submitted. As was stressed before, the same Lagrangian predicts very different solutions, with very different radii, if the particle is free or if it is bound to a Coulomb field. The solutions studied in this work are, in fact, solitary bounded waves. The whole kink must be taken to represent the electron. In a Coulomb field the kink has a radius of order 1 Å, and this must be considered as the radius of the electron itself in this situation.

If the electron is free, its nonlinear self-coupling, together with its electromagnetic self-interaction would change its localization, reducing tremendously its size to less than 0.1 fermi. It must be stressed again that this reduction takes place, in a smaller scale (from 5×10^4 fermi to 400 fermi), if one neglects the electromagnetic field of ψ . It is worthwhile studying whether this field makes the reduction much more dramatic.

As for the fourth objection, it is a difficult question. It is not the same thing to consider a classical field extending to a macroscopical domain as it is to consider another one in which the localization is microscopic. In the latter case the nonlinear effects may play a significant role, which may affect the usual arguments on this question.

6. Summary and Conclusions

We have found that the inclusion of nonlinear terms in the hydrogen atom modifies the results in order α^6 , which cannot be experimentally detected. For completeness, we should also consider the radiative corrections. As is well known, one of the most successful predictions of quantum mechanics refers

to the Lamb effect. It is related to the electromagnetic field produced by the electron field. From the point of view of nonlinear theory, this effect can be neglected, in the first approximation, because the great extension of the ψ field makes the current density very small. It is worthwhile to study this problem in a future work.

In the case of the relativistic hydrogen atom, quantum mechanics appears as the linear approximation to a nonlinear classical field theory. If this situation is general there is a kind of three-step hierarchy: nonlinear classical field theory reduces, by linear approximation, to quantum physics, whose reduction to classical mechanics through the Ehrenfest theorem is well known.

One of the main problems of quantum physics is the appearance of divergences. In particular the self-energy of a free particle turns out to be infinite. No such problem arises in nonlinear classical field theory. For instance the energy of a kink is finite as it is that of a bound state in potential theory. This is enough to make classical fields worthy of further study as a tool of elementary particle physics. It is clear that in this connection the main concept and, perhaps, the key of the problem is the soliton.

To summarize, the conclusions of this paper are as follows:

(1) The relativistic quantum mechanics of the hydrogen atom coincides, up to α^4 order, with the linearization of a nonlinear theory. The linearization is dominated by the term $\lambda(\bar{\psi}\psi)^2$; if $|\lambda|m^2 < 10^{-4}$, the nonlinear corrections to the energy are smaller than $10\alpha^6$ and decrease with increasing n , at least for $n = 1, 2, 3$.

(2) A nonlinear theory of the Dirac field has, near the linear limit, a quantumlike behavior. There is a close relation between linearization and quantization. When we linearize we can no longer determine the norm of the solutions, and we are, therefore, unable to establish an energy-frequency relation, which near the linear limit has the form

$$E = N\omega$$

where N is the norm of the field. To overcome this problem we must introduce the value of N as a constant. If $N = \hbar$, the well-known Planck relation holds. From the point of view of nonlinear theory this relation does not apply when we are far from the linear limit.

It is most convenient to study this point without the use of numerical analysis, in order to develop a mathematical theory of the linearization of nonlinear classical field theory.

(3) The preceding conclusion suggests the possibility of a dynamical determination of the Planck constant. If there exist very localized solitons in the case of nonlinear Dirac and Maxwell fields in interaction, a classical model of the electron could be attempted. The norm of these solitons would play the role of action quantum and ought to be equal to \hbar . The electron would, then, be considered as an extended particle, whose radius would depend on the particular situation considered.

Of course this determination of \hbar would only be valid for the hydrogen atom

or, at most, for atomic physics. The universality of the value of \hbar is far beyond the scope of this work.

(4) It is possible to construct a nonlinear classical model of the hydrogen atom, in which the electron is represented by a Dirac field. It is worthwhile to study the possibility of representing the transitions by means of the theory of stability of solutions of nonlinear partial differential equations. If this turns out to be possible a deterministic structure would be hidden behind the quantum world. The philosophical implications would be very important.

(5) This point of view could be extended to any kind of particles, representing them as solitary waves with different degrees of stability. Quantum mechanics would then be the linearization of a classical field theory of extended particles.

Most physicists accept today the interpretation of quantum mechanics that was established in the twenties, after long discussions between some of the most prominent scientists of the century. Bohr, Heisenberg, and a large majority of physicists were in the winning side. Einstein, Schrödinger, de Broglie and a few more lost the battle. Perhaps, the time has come to take up again the discussion, in the light of the surprising and unsuspected richness of the world of nonlinear equations.

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