The Dirac equation as a path to the concept of quanta, and its role in quantum electrodynamics

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Abstract

In this article the Dirac equation is used as a guideline to see the historical emergence of the concept of quanta, associated with the quantum field. In P. Jordan's approach, electrons as quanta result from the quantization of a classical field described by the Dirac equation. With this quantization procedure – also used for the electromagnetic field – the concept of quanta becomes a central piece in the applications of quantum electrodynamics. This does not seem to avoid the apparent impossibility of using the concept of quanta – and with it the common interpretation of quantum fields – when interacting fields are considered together as one complete system. In this article it is defended that the type of analysis that leads to so drastic conclusions is avoidable if a clear distinction is made between the mathematical framework of the theory and the particular physical models (used in the empirical corroboration of the theory) that are constructed using the theory. When dealing with models there really is no system of complete interacting fields, and what we have is a description of the interactions between distinct fields. In this situation the concept of quanta is central in the description of interacting fields, the Fock space being the natural mathematical structure that permits maintaining the quanta concept when considering the interaction between fields.

1. Introduction

Once upon a time, R. P. Feynman wrote that "we know so very much and then subsume it into so very few equations that we can say we know very little (except these equations – Eg. Dirac, Maxwell, Schrod.). Then we think we have the physical picture with which to interpret the equations. But these are so very few equations that I have found that many physical pictures can give the same equations" (quoted in Schweber, 1994, p. 407). He wrote this having in mind, mainly, the Dirac equation: $i\nabla\psi = m\psi$ (Feynman, 1961, p. 57).

In this article I will try to elaborate some 'pictures', or more exactly give some perspectives on the physical-mathematical framework related to the Dirac equation and its use in physical models developed within quantum electrodynamics, and try to get a glimpse of the 'so very much' that is condensed in so very little.

The meaning of the simple looking Dirac equation is not as simple as we might think. Since its first formulation, its meaning has changed from a relativistic wave equation for an electron to a classical field equation from which an electron-positron quantum field is derived; and from a relativistic 'update' on the Schrödinger equation in the calculation of energy levels in atoms (basically of hydrogen), it became one of the cornerstones of the most successful quantum field theory: quantum electrodynamics (section 2). To clarify the relation between the different interpretations of the Dirac equation, the results provided by Dirac's equation as a relativistic one-electron equation are reinterpreted from the perspective of the quantized Dirac field (section 3). Doing this, the importance of the concept of quanta in the description of bound states becomes clear. By contrast, bound states are usually only analyzed at the level of the one-electron interpretation of the Dirac equation, which gives a distorted idea of the physical description of bound states that should be analysed from the perspective of quantum fields. In particular, an analysis of a two-body model for the hydrogen atom reveals a

distinctive feature of quantum electrodynamics: the interaction between fermions described as an exchange of photons. A closer look at the interaction between Dirac and Maxwell fields reveals the existence of mathematical problems in the application of the theory in the description of the interaction between fields (section 4). Haag's theorem seams to render impossible the usual treatment of interaction within quantum electrodynamics using perturbative methods. To overcome the mathematical consequences of the theorem a clear separation is needed between what might appear to be the physics inscribed in the mathematical formalism of the theory and the physics that is imperfectly sustained by the mathematical formalism of the theory. It might appear (at least from a mathematical point of view) that the theory provides means to treat almost undifferentiated interacting fields. On the contrary, from a physical point of view, the theory was developed as a theory that describes the interaction between clearly distinct fields. In this way the mathematical difficulties related to the convergence problem of the series resulting from the perturbative approach used in the description of interactions (Aramaki, 1989, pp. 91-93) can be seen from the positive perspective of meaning that we have to use the mathematical formalism carefully, subjected to the physical content of the theory, not the other way around.

2. Different views on the Dirac equation

2.1. Dirac's equation as a one-electron equation

In the early days of 1928, in the paper that presented what he thought was a relativistic wave equation for one electron, P. A. M. Dirac made a clear distinction between the model of a spinning electron[1] and the simpler model of a point-like electron, which he used in the development of his equation. It seems that the spin had no direct relevance to Dirac's work (besides his 'playing' around with the mathematics that Pauli used to 'put' the spin into a Schrödinger-like equation for a two-component wave function: the Schrödinger-Pauli equation), but nevertheless it came out as a 'natural' mathematical consequence of the equation (Kragh, 1981, p. 56). But as Dirac remarks, this is a different spin from the one in the "previous electron theory" (Dirac, 1928, p. 620). So we might say, following Pauli's view on the subject, that this strange creature, the spin, is of a quantum character, a 'characteristic' of the electron which, nevertheless, Dirac regards as a point-like particle.

In his 1927 article on the quantization of the electromagnetic field, Dirac clearly stated that there was no wave – in the sense that we can consider light as a wave in space – which we might associate with the electron (Dirac, 1927b, p. 247). Regarding the Schrödinger wave equation from the point of view of his transformation theory, for Dirac "the eigenfunctions of Schrödinger's wave equation are just the transformation functions … that enable one to transform … to a scheme in which the Hamiltonian is a diagonal matrix" (quoted in Moyer, 1981, p. 946). This highly abstract approach is to be contrasted with Schrödinger's original approach where he developed his wave equation taking into account L. de Broglie's association of a wave with the electron (Schrödinger, 1926a, p. 9).

The main guidelines in obtaining Dirac's equation were, besides the requirement of being relativistic, to conform to the mathematical scheme of transformation theory. This meant an equation that is linear in the time derivative d/dt. Dirac felt that "an

[1] Referring to the model of the spinning electron, Dirac associated the different views of W. Pauli and C. G. Darwin to the more semi-classical idea of S. A. Goudsmit and G. E. Uhlenbeck, which first saw the light with R. de L. Kronig (Dirac, 1928, p. 610; Kragh, 1981, pp. 44-47; Tomonaga, 1974, pp. 32-42).

appropriate formulation of quantum mechanics will only be possible when we succeed in treating space and time as equal to one another" (quoted in Kragh, 1990, p. 54). This means that space and time must appear in the equation on equal footing, as the coordinates of a Minkowski space-time.

Dirac ended up with a relativistic equation for a four-component wave function (Dirac, 1928, p. 615):

$$[p_0 + \rho_1(\boldsymbol{\sigma}, \mathbf{p}) + \rho_3 mc]\psi = 0\,,$$

where $p_0 = i\hbar\,\partial/(c\partial t)$ and $p_r = -i\hbar\,\partial/(c\partial x_r)$ with r = 1, 2, 3; $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is a vector formed with four rows and columns matrices that are an extension of the 2 × 2 Pauli matrices, and the 4 × 4 matrices ρ_1 and ρ_3 are also obtain from the Pauli matrices (Dirac, 1928, p. 614).

Spin could account for two of the four components of the wave function solution of the Dirac equation, but there were another two that had to be accounted for.

In the simplest case of a free electron, four independent solutions exist: two corresponding to electron states with positive energy and two to states with negative energy. Dirac's first attitude was to reject these negative-energy solutions because they referred to a charge +e of the electron (Dirac, 1928, p. 618). More generally the wave function will have components corresponding to positive and negative energy, as can be seen in the application of the equation in the determination of the energy levels for an electron in motion in a central field: a model for the hydrogen atom. Dirac considered an approximate solution to this problem in which he could neglect half the components, and apparently obtain a two-component equation that "becomes the same as the ordinary Schrödinger equation for the system, with relativity correction included" (Dirac, 1928, p. 623). But when solving exactly the equation for an electron in a Coulomb potential, the upper and lower two-components of the four-component wave function are solutions of two coupled equations (derived from the Dirac equation) and so we must associate with the electron in the hydrogen atom a four-component wave equation (Dirac, 1958, pp. 269-272; Sakurai, 1967, pp. 122-129).

Dirac's not very consistent idea of neglecting the negative-energy solutions was soon challenged when O. Klein showed that the simple case of a positive-energy wave incident on a potential barrier could give rise to a transmitted negative-energy wave (Mehra & Rechenberg, 2000, pp. 309-311). More importantly, to obtain the Klein-Nishina relativistic formula for the photon-electron scattering, the negative-energy solutions had to be considered, and as N. Bohr puts it: "The striking confirmation which this formula has obtained became soon the main support for the essential correctness of Dirac's theory when it was apparently confronted with so many grave difficulties" (quoted in Kragh, 1990, p. 89). So, the existence of negative-energy solutions in the Dirac equation had to be addressed properly.

This was done by Dirac himself. He recognized the problem that "in the general case of an arbitrary varying electromagnetic field we can make no hard-and-fast separation of the solutions of the wave equation into those referring to positive and those to negative kinetic energy" (Dirac, 1930, p. 361), and proposed as a solution that "*all the states of negative energy are occupied except perhaps a few of small velocity*. […] We shall have an infinite number of electrons in negative-energy states, and indeed an infinite number per unit volume all over the world, but if their distribution is exactly uniform we should expect them to be unobservable" (Dirac, 1930, p. 362).

In this first version of his negative-energy electron sea the 'holes' in the ocean were identified as protons: "*the holes in the distribution of negative-energy electrons are the protons*" (Dirac, 1930, p. 363). A few months latter, a note by J. R. Oppenheimer

(1930) was published in which the author calculated the transition probability for the annihilation of an electron and a proton that corresponds to the filling of a hole in the sea. The result was not very promising. Oppenheimer obtained a mean lifetime of a free electron in matter that was too low (Kragh, 1990, pp. 101-102).

What turned out to be more important was H. Weyl's demonstration that "according to Dirac's own theory of the electron the hole must necessarily have the same mass as an ordinary electron" (quoted in Kragh, 1990, p. 102). This paved the way to a second version of Dirac's sea in which "a hole, if there is one, would be a new kind of particle, unknown to experimental physics, having the same mass and opposite charge to an electron. We may call such a particle an anti-electron" (Dirac, 1931, p. 61).

The reception of the 'hole' theory was not very warm. Some compared the negative-energy sea with the unobservable ether, others referred to the negative-energy electrons as donkey electrons because of their unusual 'dynamical' behaviour, and Pauli – not restrained by Dirac's views on the importance of the transformation theory – worked out with V. F. Weisskopf a quantum field theory based on the Klein-Gordon equation, in which there was no need for a sea to take care of the concept of anti-particle (Kragh, 1990, pp. 111-114). In this work they followed recent approaches where the electrons and the anti-electrons (positrons) were described in the formalism of the theory on the same footing in a completely symmetrical way (Heisenberg, 1934, p. 183; Schweber, 1994, pp. 76-77; Zinkernagel, 1998, p. 125).

This symmetrical treatment of the electrons and the positrons solved the newly created interpretation problem of Dirac's equation, because Dirac's solution of the negative-energy difficulty makes it impossible to maintain a single electron interpretation of his equation, as can be seen in the derivation of the Klein-Nishina formula using the hole theory: In the scattering of a photon by a free electron, intermediate states with a negative-energy solution must be considered. For example an intermediate state must be considered in which a negative-energy electron absorbs the incident photon and makes a transition to a state of positive-energy, leaving a hole present (that is seen as a positron). Then the free electron "drops into the hole and fills it up" (Dirac, 1930, p. 363), emitting the outgoing photon. In this intermediate state we have three particles present (Sakurai, 1967, pp. 134-138), which means that the one-electron interpretation of Dirac's equation is not consistent.

2.2. Dirac's equation as a classical wave equation: a first perspective

As Dirac himself mentioned, the appearance of negative energy solutions "is inherent in any relativistic theory. It occurs also in classical relativistic theory, but is not then serious since, owing to the continuity in the variation of all classical dynamical variables, if the kinetic energy $cp_0 + eA_0$ is initially positive … it cannot subsequently be negative" (Dirac, 1958, p. 273). So, as a classical electron-wave equation, Dirac's equation wouldn't be so problematic in what regards the presence of negative-energy solutions.

In Dirac's calculations of the motion of a particle in a central force field no explicit use of commutation relations between operators is needed, only a straightforward solution of two coupled differential equations. A similar situation occurs with the Schrödinger equation. In both cases a more classical view of the equations is possible, using them as classical wave equations whose solutions – in the simple case of one electron – are then submitted to the quantum relation $E = h\nu$ (Tomonaga, 1962, pp. 47-54, Vol. 2).

When applying the Schrödinger equation to a system of n electrons, the wave function $\phi(x_1, \ldots, x_n, t)$ depends on the 3n position coordinates of what we can call a configuration space. Because of this H. A. Lorentz in a letter to E. Schrödinger mentioned that "I cannot interpret the waves and vibrations physically" (quoted in Jammer, 1974, p. 32). Schrödinger recognized this problem when he wrote that "we must not forget that it is only in the one electron problem that the interpretation as a vibration in real three-dimensional space is immediately suggested"[2] (Schrödinger, 1926b, p. 28).

When approaching the hydrogen atom, from an electron-wave perspective (meaning using Schrödinger equation as an equation for a 'real' wave in 'real' space) the Bohr quantum numbers appear as a classical consequence of the wave properties of the electron. Considering the Schrödinger wave equation for the proper oscillation of an electron-wave in a central potential:

$$\Delta\phi + 8\pi^2 m\left(\nu + \frac{e^2}{h}\frac{1}{r}\right)\phi = 0\,,$$

we obtain for the proper frequencies of the electron-wave

$$\nu = -\frac{2\pi^2 m e^4}{h^2}\frac{1}{(n_r + l + 1)^2}\,,$$ where $n_r, l = 0, 1, 2, \ldots$ (Tomonaga, 1962, pp. 47-54, Vol. 2).

As S. Tomonaga puts it: "we have used here the terminology 'quantum number' for n, l and m. Strictly speaking this is not the proper terminology in wave theory, since these numbers are nothing but the number of nodal surfaces of the wave and have nothing to do with quantization" (Tomonaga, 1962, p. 55, Vol. 2). In the particular case of one electron the quantization 'procedure' corresponds simply to taking the energy to be a multiple of the wave frequency using the relation $E = h\nu$, so that the discrete energy levels follow directly from the classical discrete frequencies of an electron-wave 'bound' in the atom.

We can do the same to Dirac's relativistic equation for a point-like electron. In this case, Dirac's results for the electron in a central field can be reinterpreted as an application of a classical wave equation (with some 'strange' properties like ψ being a complex function as in the Schrödinger equation). The solution of this non-quantum wave equation in the case of the electron-wave subjected to a Coulomb potential gives the discrete set of frequencies from which, using the simple quantum relation $E = h\nu$, the 'correct' energy levels come out. So, in this simple scheme we would not have any commutation relations because there would not be any quantum operators.

2.3. The (classical) Dirac equation and the quantization of the Dirac field

When in 1927 Dirac developed a quantum treatment of the electromagnetic field he did this from two different approaches, which at a quantum level gave the same mathematical result. In the final part of his paper Dirac extended Jordan's initial work on the quantization of the electromagnetic field (Born, Heisenberg & Jordon, 1926; Schweber, 1994, p. 11; Darrigol, 1986, pp. 220-221). Dirac began by resolving the

[2] The recognition of this situation however did not prevent Schrödinger from developing mainly an electromagnetic electron-wave interpretation (Schrödinger, 1926c, pp. 120-123).

radiation field into its Fourier components. Then, having made the Fourier expansion of the field, "we can consider the energy and phase of each component to be dynamical variables describing the radiation field … we can suppose each E_r and θ_r to form a pair of canonically conjugate variables … satisfying the standard quantum conditions $\theta_r E_r - E_r\theta_r = i\hbar$ … this assumption immediately gives light-quantum properties to the radiation" (Dirac, 1927b, p. 244).

But the main drift of Dirac's work was not the quantization of a wave; on the contrary his paper is mainly a treatment of an assembly of identical particles. It seems that Dirac got to this approach by "playing about with Schrödinger equation" (quoted in Darrigol, 1986, p. 226). In this method, later called 'second quantization', Dirac started with an assembly of N similar independent particles subjected to a perturbation, whose wave function is $\psi_r = \Sigma_r a_r \psi_r$ (where ψ_r are the eigenfunctions of the free particles), and considered the expansion coefficients a_r as canonical conjugates. Working with the canonical variables $b_r = a_r\, e^{-iw_r t/\hbar}$ and $b_r^* = a_r^*\, e^{iw_r t/\hbar}$ (where w_r is the energy of the unperturbed state), Dirac assumed that these variables were "q-numbers satisfying the usual quantum conditions instead of c-numbers" (Dirac, 1927b, p. 251). This gives the false impression that a quantization scheme is being used, but what is being done is changing from a configuration space representation to a occupation number representation (Cao, 1997, pp. 166-167), where the commutation relation $[b_r, b_s^*] = \delta_{rs}$ holding between b_r and b_r^* serves to impose the symmetrization of the configuration space wave function, which means that the particles obey Bose-Einstein statistics (Dirac,1927b, pp. 252-255; Schweber, 1994, p. 28). What Dirac thinks he demonstrates in this work, is the equivalence between a quantized electromagnetic wave and a system of bosons (light-quanta), but for this he makes an identification of the quanta of energy with the particles (light-quanta), and in order to get this result the particle cannot cease to exist when it is apparently absorbed, or created when it is emitted. It is therefore necessary to have an infinite sea of light-quanta in a state in which their momentum and energy are zero, from which the particle can jump from or into (Cao, 1997, pp. 163-164). One thing seems clear, even in the case of the electromagnetic field, Dirac developed his work mainly from a particle perspective.

Jordan's approach was almost the opposite. He chose to see the Schrödinger equation as an equation for a classical wave that we would submit to a quantization procedure. The rupture with Dirac's view is most evident in Jordan's application of this approach to the electrons (fermions) using anticommutation relations, a view impossible for Dirac who saw the electrons as particles. Jordan clearly stated his ideas:

> The results we have reached hardly leave any doubt that … a quantum-mechanical wave theory of matter can be developed that represents electrons by quantized waves in the usual three-dimensional space. The natural formulation of the quantum theory of electrons will be attained by conceiving light and matter as interacting waves in three-dimensional space. The basic fact of electron theory, the existence of discrete electric particles, appears in this context as a characteristic quantum phenomenon; indeed it means exactly that matter waves occur only in discrete quantum states (quoted in Darrigol, 1986, p. 232).

The work of Jordan (and his collaborators) was extended by Heisenberg and Pauli in the development of a quantum theory of fields in which the electromagnetic and matter fields were described by a classical Lagrangian and quantized by a new method (Miller, 1994, p. 31). The difficulties in the quantization of the Maxwell equations delayed for more than a year the completion of their work. When finally Heisenberg managed "to eliminate the difficulties by means of a formal trick" (quoted in Pais, 1986, p. 343),

Dirac had already published his equation, and Heisenberg and Pauli adopted it in their quantum field treatment of the interaction of matter and the electromagnetic field.

After a subsequent refinement, mentioned above, the quantum field approach gave a different view on the negative-energy solutions without need for the hole theory. Taking the Dirac equation and its adjoint equation as classical field equations derived from a classical Lagrangian, an arbitrary field can be expanded in terms of the complete set of free-particle solutions. In the usual scheme for a 'box' quantization we have

$$\psi(\mathbf{x}) = \int \frac{d^3p}{(2\pi)^{3/2}} \left(\frac{m}{E_{\mathbf{p}}} \right)^{1/2} \left\{ \sum_{r=1}^{2} b_r(\mathbf{p}) w^r(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} + \sum_{r=3}^{4} b_r(-\mathbf{p}) w^r(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}} \right\}.$$

Replacing the expansion coefficients by operators satisfying the anticommutation relations $[b_n, b_m]_+ = [b_n^*, b_m^*]_+ = 0$ and $[b_n, b_m^*]_+ = \delta_{nm}$, $\psi(\mathbf{x})$ and the adjoint spinor field $\psi^*(\mathbf{x})$ become operators that act on state vectors of a Fock space[3], and $b_r(\mathbf{p})$ and $b_r^*(\mathbf{p})$ are interpreted as the annihilation and creation operator of an electron in a state characterized by ($\mathbf{p}$, r). Redefining the operators for the negative-energy states as $b_{r+2}(-\mathbf{p}) = d_r^*(\mathbf{p})$ and $b_{r+2}^*(-\mathbf{p}) = d_r(\mathbf{p})$ with r = 1, 2, these operators can be interpreted as the creation and annihilation operators for a positive-energy positron (Miller, 1994, p. 183), and the expansion of the $\psi(\mathbf{x})$ operator is now given by

$$\psi(\mathbf{x}) = \int \frac{d^3p}{(2\pi)^{3/2}} \left(\frac{m}{E_{\mathbf{p}}} \right)^{1/2} \sum_{r=1}^{2} \left\{ b_r(\mathbf{p}) w^r(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} + d_r^*(\mathbf{p}) v^r(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{x}} \right\}$$ (Schweber, 1961, p. 223).

With this formulation there are no negative-energy states (identified as the positive-energy positrons), and so no need for the infinite sea of negative-energy electrons. Also in the field operators $\psi(\mathbf{x})$ and $\psi^*(\mathbf{x})$ we have simultaneously operators related to electrons and positrons: they are both a manifestation of the field.

Considering the energy-momentum operator

$$P^\mu = \sum_r \int d^3p\, p^\mu [a_r^*(\mathbf{p}) a_r(\mathbf{p}) + b_r^*(\mathbf{p}) b_r(\mathbf{p})] = \int d^3p\, p^\mu [n^-(\mathbf{p}) + n^+(\mathbf{p})],$$

and the total charge operator

$$Q = \sum_r \int d^3p [-a_r^*(\mathbf{p}) a_r(\mathbf{p}) + b_r^*(\mathbf{p}) b_r(\mathbf{p})] = \int d^3p [n^+(\mathbf{p}) - n^-(\mathbf{p})],$$

where $n^-(p)$ is the number of the quanta denominated as electrons and $n^+(p)$ is the number of quanta denominated as positrons (Jauch & Rohrlich, 1976, p. 64), the quantization of charge and subsequent emergence of a particle-like concept of an electron can be seen as a result of the quantization of the classical field, as Jordan proposed.

[3] Considering the vacuum state, which is the state with no quanta, an n-quanta Hilbert space can be defined by n applications of creation operators. The Fock space is the (infinite) product of the n-quanta Hilbert spaces: $H^{(0)} \oplus H^{(1)} \oplus H^{(2)} \ldots$ (Schweber, 1961, pp. 134-137).

3. Combining results from the different views on Dirac's equation

3.1. A quantized electron-positron field view on the solutions of the Dirac equation as a relativistic one-electron equation

To connect the electron-positron quantum field with Dirac's view of electrons (and positrons) as particles, we might proceed like he did in the case of the electromagnetic field – considering the idea of light-quanta – and try an 'electron-quanta' view. In this case we would end up considering that "the Dirac equation in the quantized theory should be regarded as a differential equation that determines the dynamical behaviour of the entire aggregate of electrons (and positrons)" (Sakurai, 1967, p. 148). Even in this more favourable attitude towards a particle view of the electron, it is clear that in the field operators there is a clear separation between the components related to the electrons and the ones related to the positrons.

In the exact solution of the one-electron Dirac equation in a central potential (the hydrogen atom) we see in the new field (or aggregate) perspective components related to both electrons and positrons. This means that the one-electron four-component wave solution must be reinterpreted by taking into account the field perspective that clearly relates the positive-energy solutions to the electrons and the negative-energy solutions to the positrons. Also, if we want, from this perspective, a simple model for the hydrogen atom with only one electron, using the Dirac equation as a relativistic one-electron equation, we must have some other way of doing the calculations, or, what is the same, of creating a model that uses only two-component positive-energy wave functions to describe the electron. This approach is also important if we want to make a clear connection between the relativistic and non-relativistic equations, that is, between the Dirac and the Schrödinger equations.

Considering the positive-energy four-component solutions of the Dirac equation: $u_+ = (u_+^L\ u_+^S)$, in the non-relativistic limit the lower two components u_+^S are smaller than the upper two u_+^L. When calculating matrix elements like $(u_+, \gamma_4 u_+) = u_+^{L*}u_+^L - u_+^{S*}u_+^S$, neglecting terms of order $(v/c)^2$, we consider only the large components $(u_+^L, u_+^L) = u_+^{L*}u_+^L$ that corresponds to a two-component wave function (Mandl, 1957, pp. 214-215). In the presence of electromagnetic coupling the large components can be seen as the solution of the Schrödinger-Pauli non-relativistic two-component wave equation (Björken & Drell, 1964, pp. 10-13).

Concerning this approach to the problem of the non-relativistic limit of the Dirac equation, L. L. Foldy and S. A. Wouthuysen considered that "the above method of demonstrating the equivalence of the Dirac and Pauli theories encounters difficulties […] when one wishes to go beyond the lowest order approximation" (Foldy & Wouthuysen, 1949, p. 29). In the case of the Dirac equation for a free electron it is possible to perform a canonical transformation on the Hamiltonian that enables to uncouple the positive- and negative-energy components of the wave equation. This means we get two independent equations for two-component wave functions, and identify the equation with positive-energy solution as the Schrödinger-Pauli equation. The case of an electron interacting with an external electromagnetic field is more involving. The trick is to consider the electromagnetic field as a perturbation and to make a sequence of transformations to obtain the separation of negative- and positive-energy solutions (corresponding each to two-component wave functions). In the non-relativistic limit, like in the previous method, the Schrödinger-Pauli equation is obtained.

It is then possible to rework the relativistic Dirac one-electron equation in a way in which only the positive-energy solutions are considered, including the case of the hydrogen atom. Foldy and Wouthuysen applied their method to the case where a Dirac electron interacts with an external electromagnetic field, and obtained, making three canonical transformations and using only terms of order $(1/m)^2$, the same results as the Pauli-Darwin semi-empirical theory – as Dirac did in is original work –, but making a clear separation of positive- and negative-energy solutions using directly a two-component wave equation.

3.2. A Dirac field approach to the hydrogen atom

One of the most relevant aspects in the construction of a hydrogen atom model using only positive-energy solutions is that it is only an approximate approach, and that, moreover, it is not possible to make an infinite sequence of transformations to get the exact solution. An infinite sequence of canonical transformations leads to a Hamiltonian which is an infinite power series, and, as Foldy and Wouthuysen remarked, "it can hardly be expected that this series is convergent, the series is presumably an asymptotic or semi-convergent series in the sense that the sum of a finite number of terms of the series is a better-and-better approximation" (Foldy & Wouthuysen, 1949, p. 34). This means that a hydrogen atom model with one positive-energy electron is poorer than the previous calculation with the positive- and negative-energy components mixed up.

This takes us to the necessity of making a derivation of a quantum field model for the hydrogen atom as exact as the one-electron four-component eigenfunction calculation. One of the approaches is to use the so called Furry or bound interaction representation within the external field approximation. This gives a method for calculating corrections to the energy levels of a bound electron determined by the Dirac equation as a relativistic one-electron equation (Berestetskii, Lifshitz & Pitaevskii, 1982, p. 487). But the starting point is the field operator defined by

$$\psi(x) = \sum_{\mathrm{r}} u_{\mathrm{r}}(\mathbf{x}) a_{\mathrm{r}} e^{-\mathrm{i}E_{\mathrm{r}}t} + v_{\mathrm{r}}(\mathbf{x}) b_{\mathrm{r}} * e^{\mathrm{i}E_{\mathrm{r}}t},$$

where $u_r(x)$ and $v_r(x)$ are obtained by solving the Dirac equation for a positive-energy particle representing the electron, and a negative-energy particle representing de positron: $Hu_a(x) = E_a u_a(x)$ and $Hv_b(x) = -E_b v_b(x)$, where $H = i\gamma^0\boldsymbol{\gamma}.\nabla - e\gamma^0\gamma_\mu\varphi^\mu + i\gamma^0 m$, with φ^μ a static external field (Jauch & Rohrlich, 1976, p. 313). The first equation is exactly the one solved in the case of the one-electron interpretation of the Dirac equation. This means that E_a gives the energy levels obtained by this method, and that in spite of identifying $u_a(x)$ as the electron's wave function it contains positive- and negative-energy components (Schweber, 1961, p. 566).

Now, what is needed is a method in which the free particle positive-energy characteristic of the electron is maintained during the interactions with no mixing of positive- and negative-energy components. This implies seeing, at the quantum field level, the binding of an electron as resulting from the scattering of the electron by an external field.

The main working tool in quantum electrodynamics, the S-matrix, was designed for scattering problems where we have free particles in the beginning and free particles in the end of an interaction (scattering). This means that it is not very appropriate to deal with the case of a bound particle, at least in a direct way. On the other hand, one of the most important characteristics of quantum field methods is that the interaction between

fermions is represented by the exchange of quanta of one field by the quanta of another (Zee, 2003, p. 27). For example the electron-electron scattering is simulated by the exchange of photons between the electrons. If we make a model of the atom in which the effect of the nucleus is simulated by a classical Coulomb field, this view is lost (as in the external field method previously discussed). A way to overcome these difficulties is to address directly the two-body problem using the Bethe-Salpeter equation. The two-body problem is addressed in this method by considering directly the two-particle propagator for an electron and a proton (that in the calculations is modelled as a 'big' positron with the same mass as the proton)[4]. Considering a power series expansion of the two-particle propagator, the binding energy between a proton and an electron is basically calculated using what is known as the ladder approximation (Schweber, 1961, p. 713). Concerning this approximation H. A. Bethe and E. E. Salpeter considered that "although the probability for the exchange of a quantum during a small time interval is fairly small, during the infinite time of existence of the bound state an indefinite number of quanta may be exchanged *successively*. It is just such processes that the ladder-type graphs deal with" (Salpeter & Bethe, 1951, p. 1234). Thus, in the field theory model the binding of the electron in the atom is achieved by an exchange of photons with the proton. We see that from a field theory perspective, a rigorous description of the hydrogen atom (as a two-body problem) leads to a physical picture of the process going on in the atom quite different from the one obtained when using the Dirac equation as a one-electron equation.

4. Interacting fields or interaction between fields

4.1. Interacting fields and theory design in quantum electrodynamics

From a Jordan's perspective on quantization of a classical field, the eigenfunctions of the field operator are a superposition of classical field configurations (Schweber, 1961, p. 193). In this case we can see the Fock space as constituted by the "wavefunctionals $\psi(\phi)$ that describe superpositions of different classical field configurations" (Baker, p. 5). This means that we can construct the Fock space associating classical field configurations to the field quanta.

The analysis of the theory in terms of a field interpretation of the Fock space, and the use of the quanta concept in the description of fields and their interaction might be thrown over board when we make a detailed analysis of the mathematics of the interacting system of Dirac and Maxwell fields. Since as seen before, apparently, the interaction has a physically appealing description in terms of quanta exchange – or more properly, coordinated creation and annihilation of quanta of the two fields – at first sight it looks strange that from a deeper analysis of the interaction (the important stuff) we might get into trouble.

Using the Lagrangian formalism, in quantum electrodynamics, the system of interacting Dirac and Maxwell fields is described by a Lagrangian $L = L_0(A_\mu) + L_0(\psi) + L_I(\psi, A_\mu)$, where $L_0(\psi)$ and $L_0(A_\mu)$ are the Lagrangian densities for the free Dirac and Maxwell fields, and $L_I(\psi, A_\mu) = e\overline{\psi}\gamma^\mu\psi A_\mu$ is the interaction term. The form of the latter term can be determined by imposing invariance requirements on the total Lagrangian

[4] There is an indirect method to calculate the energy levels of bound states from the S-matrix, which consists in determining the poles of the exact scattering amplitude. But in practice this approach leads to a summation of an infinite series of diagrams that corresponds to solving the Bethe-Salpeter equation (Berestetskii, Lifshitz & Pitaevskii, 1982, p. 554).

and selecting the simplest expression possible. The interaction term can also be obtained by correspondence to the classical term in the Lorentz theory of electrons.

Considering the relativistic equation of motion for an electron in an external field A_μ (basically the four-vector version of the Lorentz force law), a Hamiltonian is defined using the total four-momentum of the electron: $p_\mu = u_\mu + eA_\mu$ (Heitler, 1954, p. 15). From the Hamilton equations, the expression for the equation of motion is derived with the 'kinetic momentum' being given by $u_\mu = p_\mu - eA_\mu$ (Heitler, 1954, p. 43), which corresponds to the minimal coupling used in quantum electrodynamics.

The variation of the Lagrangian with respect to the field operators results in a set of nonlinear coupled equations. In this case, the Dirac equation in the presence of the electromagnetic field is given by $i(\not\partial - e\not A)\psi = m\psi$ (Feynman, 1961, p. 56).

It is relevant that quantum electrodynamics, as an interacting field theory, is designed as a theory that describes the interaction between distinct fields. Quantum electrodynamics was developed by considering two clearly separated fields from the beginning, which corresponds to having in the Lagrangian (the mathematical core of the theory) two separated pieces exclusive of each field. The relations between the two fields are determined by an interaction term that couples the Maxwell and Dirac equations.

The (apparent) problem we have in the case of interacting Dirac and Maxwell fields is simply that it is not possible to "use the Fock representation for a free field to represent an interacting field" (Earman & Fraser, 2006, p. 322). In the Fock space we have a direct connection of quanta to the normal modes of classical field configurations. It is from the Fourier splitting of a classical wave into positive and negative frequency normal modes, providing the basis for the configuration space, that the concept of quanta emerges (via a quantization procedure and associated to each normal mode). In the case of interacting fields it is not possible to make this Fourier expansion (Fraser 2006, p. 136). This means that following this line of reasoning the quanta concept is unavailable when we consider full interacting fields (Earman & Fraser, 2006, p. 330). Going deeper into this, it is possible to conclude that "no space of wavefunctionals over interacting fields exists, since no Fock space over such fields exists. So whatever an interacting state is, it is manifestly not a probability distribution over classical field configurations" (Baker, p. 24). This means that we would lose the concept of quanta and the field interpretation in one struck.

This problem comes about because of the differences between the practice in physics with concrete models worked out from the theory, and the mathematical abstract framework itself. The previous apparent conceptual collapse is due to that.

Even when we are not considering the incompleteness of quantum electrodynamics – in what regards the need for classical theory to construct the quantum structure as a physical-mathematical upgrade of classical physics, and also the complicated matter of the need of a classical basis for the description of observation of quantum systems – the theory does not provide the possibility of describing a closed system of interacting fields even if considering the mathematical framework of the theory it would appear it does. I consider that the previous apparent conceptual collapse results from dealing with the theory in a more abstract mathematical way and not considering the concrete applications that permit the empirical corroboration of the theory. For good or for bad, physical theories (at least the ones under consideration) have been constructed based on the idea that there can be a clear distinction between phenomena (like the distinction between matter and radiation), and that this empirical distinction can be reflected in the design of the theories. This world view of a reality built by disconnectable entities is used in quantum electrodynamics, inherited from the classical theories. The theory was

built by explicitly considering completely disentangled 'building blocks' of reality, in the present case the Dirac and Maxwell fields that exist in a Minkowski space-time. Then from the interaction of this distinct 'elements of reality' the change in the world can be 'explained'.

The trick in quantum electrodynamics is that it is not as a full interacting theory that results are worked out. If we do not bring the mathematical structure of the theory to the level of specific physical models, that can be contrasted with experimental results, but try to take a more formal approach from the general framework of the theory, not taking too much into account the physical basis of its development and its applications, we get absurd conclusions (as will be seen in the next section when considering the implications of Haag's theorem). We must analyse the interaction of fields from the perspective of independent fields that make sense on their own. Then, from the modelling of the interaction using the mathematical structure provided by the theory, results can be obtained for a system of different interacting fields, not the other way around.

4.2. From a theory of interacting fields to models of interaction between fields

The (apparent) impossibility of using the Fock space (connected with the concept of quanta) in the description of interacting fields appears as a rigorous mathematical consequence of the Haag theorem, which is valid in the context of quantum electrodynamics.

From Haag's theorem (Haag, 1955) we know that we cannot have a unitary transformation relating the field operators corresponding to the free Hamiltonian H and the interacting field Hamiltonian H_I. Considering that at t_0 the Heisenberg representation and the Dirac (interaction) representation coincide (Earman & Fraser, 2006, p. 320), in the limit $t \to \pm\infty$ it would seem that the state vector in the Dirac representation corresponds to free particles due to the fact that the interaction part of the Hamiltonian is neglectable. But from Haag's theorem it seems that "at times $t = \pm\infty$, all the assumptions of the theorem hold for the Heisenberg representation, which represents an interaction, and for the interaction representation, which is a Fock representation for a free system" (Earman & Fraser, 2006, p. 322). In informal terms Haag's theorem implies that the state vectors in the Dirac representation, that for $t \to \pm\infty$ are *supposed* to represent the free field, and the state vector in the Heisenberg representation for the interacting fields, are not in a common domain of both H and H_I (Schweber, 1961, p. 416).

From Haag's theorem we can conclude that when using the Dirac representation (also called interaction picture) in describing the interacting fields, if we have a free field at $t = -\infty$, the Dirac representation describes also a free field at any time t_0. This means that we need from the start to have a state of the full interacting Hamiltonian so that we can consistently give to the Dirac representation its usual use in giving a different time dependency to the state vector and the operators (Schweber, 1961, p. 317).

Both the Heisenberg and Dirac representations can hypothetically be used in free or interacting systems, if we can separate in parts the Hamiltonian corresponding to free fields and an interaction term. The change of representation does not change the physical situation, be it of free fields or interacting fields. The change of representation does not bring a magical change from free fields to interacting fields or vice versa. There really is no "interaction picture's assumption that there is a time at which the representation for the interaction is unitarily equivalent to the Fock representation for a

free system" (Fraser, 2006, p. 54). This 'assumption' has nothing to do with the representation being used. The 'assumption' is that with an adiabatic switching of the interaction, the state vector for the interacting systems can be constructed from the state vector of free fields (Schweber, 1961, p. 320):

$$\lim_{t\to-\infty} U(t_0,t)\left|\varphi_a\right\rangle = \left|\psi_a\right\rangle .$$

This is what is supposed to be achieved in the adiabatic switching of the potential that 'connects' a free field Hamiltonian with the interacting field Hamiltonian (Jauch & Rohrlich, 1976, p. 134; Schweber, 1961, p. 322):

$$\lim_{t\to-\infty} H_\varepsilon(t) = \lim_{t\to-\infty}(H_0 + e^{-\varepsilon|t|}V(t)) = H_0 .$$

The point is that at infinite times before and after the adiabatic switching of the interaction potential, the state vector in the Heisenberg or Dirac representation is assumed to be describing free fields.

The question here is not the representation being used but when, how, and whether, it is possible to connect the interacting state to a free field state. It seems clear from the consequences of Haag's theorem that the usual adiabatic switching of the interaction won't do the trick.

It might seem that by using renormalization techniques the consequences of Haag's theorem might be evaded because "once infinite renormalization counter terms are introduced, the interaction picture is not mathematically well-defined" (Fraser, 2006, p. 2), and from this it might seem that "renormalization addresses this problem not by refining the assumptions, but by rendering the canonical framework mathematically ill-defined" (Fraser, 2006, p. 90). We would be in the surrealistic situation of needing bad maths to get good physics. But it would be rather strange to say the least, that considering an impoverished mathematical framework, suddenly, something physically equivalent to a unitary transformation connecting free and interacting field operators might emerge.

There does not seem to be any relation between the functionality of the Dirac representation in scattering problems in spite of Haag's theorem, and the necessity of mass and charge renormalization to render the results finite (a problem that is not addressed here).

The explanation for the good results of the perturbation theory approach to the scattering (and bound state) problems will not be found in the inapplicability of Haag's theorem in the ill-defined mathematical framework of quantum electrodynamics. It is not in the mathematical imperfections of the theory that we should look for an answer to the functionality of the theory despite Haag's theorem. We must look for a physical justification of it, even if this involves (as it is the case here) a clear imperfection in the mathematics of the theory as it is used. To properly address this question we have to work at the level of physical models.

The use of the Dirac representation only makes physical sense at the level of models in which we can consider different systems (described by a limited number of quanta) that have some sort of interaction we can consider as a perturbation to their independent states, in this way maintaining their identity as separated physical systems even during the interaction. In this sense the use of Dirac representation is part of the model design. We simply use part of the Hamiltonian, which is possible since the theory was developed considering distinct parts in the Lagrangian, one corresponding to the free

Dirac field, another to the free Maxwell field and another to the interaction. This is the one pulled apart from the others in the Dirac representation.

The model for scattering is constructed from the theory considering an initial state corresponding to a limited number of free particles (quanta), and with an adiabatic switching of the interaction between the fields, a full interacting state ψ_b^- is *apparently* obtained. The interacting state ψ_a^+ that corresponds to a determined number of quanta in the final state is defined in an equivalent way. The scattering amplitude S_{ab} is given by (ψ_b^-, ψ_a^+) (Schweber, 1961, p. 323).

The point is that we really do not work with this doubtful interacting state. What is going on is quite different. We are only considering the first terms of a perturbation expansion of the scattering matrix corresponding to particular cases of quanta present. At the model level we are taking advantage of the way the theory was designed. We always have clearly distinct fields, and for the description of their interaction, with an excellent agreement with experimental results (Gabrielse et al., 2007), a blending of the description of the fields as a global interacting system is not needed. On the contrary, if we try to make a full description of the interaction considering all the (infinite) terms of the power series expansion of the S-matrix there is good reason to believe that in the present theory this series can "at best only be an asymptotic expansion" (Schweber, 1961, p. 644).

From a mathematical point of view the use of a few terms of a divergent series is difficult to defend, but from a physical perspective the justification for the use of perturbation theory in quantum electrodynamics is clear. It is related to the weakness of the interaction between the Maxwell and Dirac fields (Mandl & Shaw, 1984, p. 95). The possibility of a perturbative approach is a mathematical fingerprint of the physical distinction between the fields in the interpretation of all the experimental results that are agreed by the models of the theory.

If when calculating the amplitude, for example, for the electron-electron scattering, the complete S-matrix was (somehow) considered, then there would be an infinite number of terms corresponding to an infinite number of combinations of different quanta, and we could say that in this case the quanta "type and number are not sharp" (Weingard, 1988, p. 46). The quanta description of interactions would then appear to be a mathematical fiction due to the use of perturbation theory in the calculation of the scattering amplitude. Simply, when considering a model of the scattering, we can only use the first terms of the S-matrix expansion. There is simply no possibility of considering the (unexisting) exact S-matrix, nor is there a motive[5]. We are working at the level of models of interaction between fields, not the mathematical abstract framework of the theory. In this way we are not restricted by Haag's theorem – and so we can retain the concept of quanta in the description of interactions – because, from a physical point of view, the Lagrangian of quantum electrodynamics does not provide us (contrary to what from a mathematical abstract point of view might appear) with the possibility of describing a system of (undifferentiated) interacting Dirac and Maxwell fields, but with a way of developing models that describe in a limited way the interaction between the fields[6]. This limited possibility of the theory in describing the

[5] There might appear to be ways of sidestepping this type of approach considering the Feynman path integral approach (Weingard, 1988, p. 54). But again, when considering the specific models there is no infinite expansion of the transition amplitudes. In the mathematical expression for the transition amplitudes there are quanta propagators, and the interpretation of the propagators relating them to quanta cannot be overturned in a (finite expansion) model based on path integrals.

[6] In this way, due to the ill-defined mathematics of quantum electrodynamics, the models are much more constructed from the theory than simply an application of it. But the models are developed within the

interaction between Dirac and Maxwell fields can be seen as an intrinsic limitation of a quantum treatment of the interaction, as Bohr stressed (Rueger, 1992, pp. 317-318). According to Bohr's views, the correspondence principle implies that the quantum treatment of the interaction of the electron with the electromagnetic field can only be treated by an "essentially approximate procedure" (quoted in Rueger, 1992, p. 318). In this way, this physical limitation can be seen to have a sort of mathematical correspondence in the convergence problems of the S-matrix and the need of the adiabatic switching on/off trick. But, it cannot be seen as resulting from the mathematically ill-defined perturbative approach. On the contrary, the mathematical imperfections should be seen as a fingerprint of an intrinsic physical limitation of quantum electrodynamics.

From the start the theory was not developed to treat the question of fully interacting almost undifferentiated fields, but to treat the question of interaction between distinct fields. To consider that "Fock representations are generally inappropriate for interacting fields" (Earman & Fraser, 2006, p. 330), is to turn upside down the theory as it was developed. The theory is built on top of the physical idea of independent entities whose interaction describes change in nature. When accepting this approach, and its intrinsic limitations, it is difficult to consider inappropriate, at least from an empirical point of view, the results of quantum electrodynamical models.

Conclusions

Accepting the construction limitations of quantum electrodynamics, it is not possible to analyse its basic physical concepts disregarding the way the theory is confronted with experimental results. The concept of quanta follows naturally from the quantization of the Dirac (and Maxwell) classical field as described by Dirac's equation, and it is fundamental for the intelligibility of the theory independently of any ontological positioning. It is a central concept in the physical-mathematical description of interaction between fields, and in the visualization and mental comprehension of what's going on at the level of physical models of interaction between fields.

In what regards quantum electrodynamics, Fock space does its job well, both for free and for interacting fields. Taking into account the evident shortcomings of the theory in the description of interactions between fields, a view of quantum electrodynamics as a full interacting field theory should not be enforced, and lead to ontological debates on the clearly limited physical concepts being used (like the concept of quanta or quantum field). The delimitation and clarification of the theory shortcomings should instead help in the development of improved theories.

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physical-mathematical framework of the theory, taking into account very basic physical ideas like the existence of two distinct fields that interact via a weak coupling constant.

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