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From quantum electrodynamics to mean-field theory: I. The Bogoliubov–Dirac–Fock formalism

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Abstract. A relativistic mean-field theory for interacting Dirac particles in an external field is derived from quantum-field theory using a minimisation principle, and discussed in the context of atomic physics. In this approach, electrons and positrons are treated on the same footing, and neither final 'reinterpretation' nor 'positive energy projection' are needed. We obtain mean-field equations of Dirac–Fock type containing a vacuum polarisation term that does not exist in the standard Dirac–Fock equations. However, the standard Dirac–Fock equations, as well as the equations resulting from earlier attempts to build a mean-field theory from quantum electrodynamics, are recovered as non-variational approximations. The minimisation principle also leads to a new way of introducing finite-basis relativistic calculations.

1. Introduction

The first relativistic mean-field theory, referred to as Dirac–Fock (DF) theory, has been introduced in 1935 (Swirles 1935) in the context of atomic physics as a mere transposition of the Hartree–Fock (HF) theory. The HF equations can be deduced from the non-relativistic Hamiltonian theory for N-particle systems through the minimisation of energy in the space of the Slater determinants $|\varphi_{HF}\rangle$ of N one-particle wavefunctions:

$$E_{HF} = \mathrm{Min}\langle\varphi_{HF}|\sum (T_a + \Omega_a + V_{ab})|\varphi_{HF}\rangle \tag{1.1}$$

where T_a and Ω_a are the kinetic and potential energies for the ath electron and V_{ab} is the interaction between the ath and bth electrons. In the relativistic context, the DF equations are usually written as a stationarity equation:

$$\delta E_{DF} \equiv \delta\langle\varphi_{DF}|\sum (h_{Da} + \Omega_a + V_{ab})|\varphi_{DF}\rangle = 0 \tag{1.2}$$

where $|\varphi_{DF}\rangle$ is an N-electron Slater determinant of normalised one-electron bispinor wavefunctions and $h_{Da} \equiv \boldsymbol{\alpha}\cdot\boldsymbol{p}_a + \beta m$ is the free Dirac Hamiltonian for the ath electron.

Relativistic effects in atoms and molecules have stimulated much interest during the past 20 years, and the DF equations have been developed into a powerful tool for the calculation and analysis of ionic, atomic and molecular relativistic structures (Kim 1967, Grant 1970, Lindgren and Rosen 1974). The improvements of numerical techniques and computer capabilities have made possible a complete numerical treatment of the DF equations, involving for instance their discretisation on a spatial lattice (Desclaux 1973), or the use of a finite-basis approximation where the one-electron wavefunctions are imposed to belong to a given finite-dimensional space (Quiney *et al* 1987). Very accurate calculations are now currently performed, which take into

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account not only the Coulomb repulsion between the electrons but also more sophisticated effective interactions derived from perturbative quantum electrodynamics (QED) (Gorceix *et al* 1987, Indelicato *et al* 1987).

Despite this success, the DF theory conveys shortcomings arising from the fact that the free Dirac Hamiltonian $h_D \equiv \boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m$ is not bounded below. These deficiencies raise questions about the meaning and the foundations of the DF theory. First, a normalised DF state cannot approximate a bound state of the Hamiltonian $\Sigma(h_{Da}+\Omega_a+V_{ab})$, since one knows that this Hamiltonian has no normalisable bound states. This 'phenomenon' is known as continuum dissolution (Brown and Ravenhall 1951, Sucher 1985). Secondly, the DF theory fails when the external potential becomes so strong that one or more bound states lie very deep in the mass gap or dive in the negative energy continuum of the DF Hamiltonian, as might happen for instance in 'over-critical' atoms (Reinhard *et al* 1971). Finally, since the expectation value E_{DF} of the N-particle Hamiltonian $\Sigma(h_{Da}+\Omega_a+V_{ab})$ has no minimum, the ground state of an atom cannot be viewed as (or approximated by) a state minimising E_{DF}. The DF equations are only stationarity equations, and this implies a new difficulty in their implementation via the finite-basis method: the finite-basis DF energy does not necessarily converge from above to the exact DF solution, if it converges at all, and its accuracy cannot be improved by a mere minimisation. Unless specific precautions are taken, e.g. constraints on the basis sets, this feature leads to 'variational collapse' and to the emergence of 'spurious states' ('finite-basis disease') (Wallmeier and Kutzelnigg 1981, Schwarz and Wallmeier 1982, Stanton and Havriliak 1984). A careful analysis of the finite-basis treatment of the DF equations (Grant 1986) made it possible to overcome these difficulties, and finite-basis DF calculations are now currently performed with the same very high accuracy as that achieved by finite-difference methods (Quiney *et al* 1989).

However, fundamental difficulties of interpretation related to 'negative energy states' remain. Since QED is believed to be the 'true fundamental theory' for electrons, it should be used to establish the DF theory on firm grounds, and therefore should provide the solutions to the above-mentioned problems. Variational collapse, spurious states and continuum dissolution result from the unboundedness of the Dirac Hamiltonian $\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m$, a feature that disappears from QED through Dirac's reinterpretation of the vacuum. QED involves no negative kinetic energy states, and its Hamiltonian is bounded below (at least it is supposed to be so, for the interaction may affect this boundedness). Therefore, an energy minimisation procedure dealing with the QED Hamiltonian is legitimate, while an energy minimisation procedure with the Dirac Hamiltonian is not. However, an additional complexity arises from the fact that QED is a many-body theory: its Hamiltonian commutes with electric charge but does not conserve the number of particles. This raises the following general question. On the one hand, QED is a relativistic quantum-field theory, and deals with Fock states and particle-number non-conserving Hamiltonians; on the other hand, DF theory is a mean-field theory, and deals with wavefunctions for a given number of particles and configuration-space Hamiltonians. How can we then deduce the DF theory from QED?

There is at present no complete answer to that question. An approach that has been considered (Brown and Ravenhall 1951, Sucher 1980, 1985) consists of splitting the Hamiltonian into a particle-number conserving part and a particle-number non-conserving part. The latter has to be treated via perturbation theory, while the former is treated variationally with Slater determinants of positive energy states. This prescription introduces positive energy projection operators Λ^+ and leads to a projected configuration-space Hamiltonian of the following form (repeated indices are summed

over):

$$h_{\text{proj}} = \Lambda_a^+(h_{Da} + \Omega_a)\Lambda_a^+ + \Lambda_a^+\Lambda_b^+(V_{ab})\Lambda_a^+\Lambda_b^+. \tag{1.3}$$

Indeed, this approach is based on QED, and therefore does not suffer from the troubles plaguing usual DF calculations. However, it does not bridge the gap between QED and the successful standard DF calculations, which do not make use of projection operators. Attempts have been made to show that one can 'optimise' the projection operators Λ^+, and that this optimisation leads to replacing them by self-consistent projection operators upon eigenstates of h_{proj} itself. Actually, this corresponds to the standard implicit prescription consisting of filling the 'physically meaningful' states only (i.e. the states with a positive eigenvalue). Although one can argue for this procedure (Mittleman 1981), it is not free from ambiguities.

We present an alternative approach to cover the distance between QED and DF theory and, more generally, between a quantum-field theory and its mean-field approximations, whatever the interaction. This approach allows one to treat variationally the whole QED Hamiltonian, including its particle-number non-conserving terms, and to recover the usual DF procedures either as restrictions or as approximations. This last feature is very important since standard DF calculations give very good results in a large range of situations. Moreover, this approach also gives a new insight into the 'finite-basis disease', and allows one to build safe finite-basis approximations. Furthermore, besides setting the standard DF method on solid grounds, our approach leads to a mean-field theory that has a broader domain of validity than the standard DF theory. For instance, it may be appropriate for the study of QED in strong external fields, or more generally for the study of non-perturbative effects in QED.

In contrast with the 'positive energy projected theory', we look for minima of the energy among variational Fock states that have definite charges but may contain virtual electron–positron pairs. Although these Fock states *do not* have definite numbers of particles, the Ritz minimisation procedure will lead to a mean-field theory.

The tool of key importance that we use is the 'Bogoliubov transformation'. This transformation has been introduced in (non-relativistic) statistical, condensed matter and nuclear physics, since it is appropriate to the study of superconductivity or superfluidity phenomena (Bogoliubov 1958, Bardeen *et al* 1957, Decharge and Gogny 1980, Ring and Schuck 1980, Abrikosov *et al* 1963). Although our perspective is quite different, the Bogoliubov transformation is still suitable because it can be shown to be the unitary transformation that diagonalises exactly one-body potentials in a relativistic fermion Fock space. As an illustration one can consider for instance an academic model in which the interaction has the form of a mass shift δm. The Bogoliubov transformation allows one to diagonalise straightforwardly the total Hamiltonian in Fock space, and dresses the particles with particle–antiparticle pairs, leading to 'dressed particles' with a mass shifted by δm (that is to say that the spectrum of the dressed particles labelled by the momentum $\boldsymbol{k}$ becomes $[\boldsymbol{k}^2+(m+\delta m)^2]^{1/2}$ instead of $\omega_k \equiv (\boldsymbol{k}^2+m^2)^{1/2}$). In a more general situation, the relativistic Bogoliubov transformation will lead to a 'dynamical dressing' of the physical particles. It must be stressed that the interpretation assigned here to the Bogoliubov transformation is different from that given within the theories of superconductivity or superfluidity, where the Bogoliubov transformation is introduced to express the production of Cooper pairs and the mean-field contributions of attractive channels in the two-body interaction.

The paper is organised as follows. Bare electrons and positrons are defined in the standard way (§ 2), and used to build the Fock space of QED in the Schrödinger picture.

Then, we introduce the Bogoliubov transformation in Fock space, and the corresponding quasiparticles, which are referred to as Bogoliubov or dressed particles (§ 3). The definition of the dressed particles leads to the introduction of the corresponding Bogoliubov or dressed vacuum, which can be interpreted as a polarised vacuum. Then an atom, or any system of electrons and positrons, is described by an independent-particle Bogoliubov state with definite numbers of dressed electrons and dressed positrons. These Bogoliubov states form a variational space in which we minimise the energy functional or look for its stationary points (§ 4). Exactly like in non-relativistic Hartree-Fock theory, this procedure leads to mean-field equations that we denote 'Bogoliubov-Dirac-Fock' (BDF) equations. The BDF energy and the BDF mean field contain new vacuum polarisation terms that do not exist in the standard DF theory. It is crucial to note that, although they are negligible in the usual domain of use of DF theory, the vacuum contributions are unavoidable if one wants to deal with a bounded-below energy functional and if one wants to remain within a minimisation procedure. Therefore, it will be necessary to take the vacuum contributions into account for the study of collapse problems and of physical situations where standard DF theory breaks down. Next, we show (§ 5) how a mere restriction of the BDF variational space leads to recovering configuration-space Hamiltonians with explicit positive energy projection operators Λ^+, and how usual DF equations are recovered by neglecting the vacuum polarisation terms in the BDF equations. Finally, we discuss in § 6 the finite-basis approximation. We show how this approximation can naturally be introduced in the Fock space, *before* deriving the stationarity equations, a procedure that differs from the usual one.

2. Fock space for electrons and positrons

One of the main features of relativistic atomic physics is that the kinetic energy of the electrons is described by the free Dirac Hamiltonian $h_D \equiv \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m$, which is not bounded below. This unboundedness renders Dirac's reinterpretation necessary. The consequence is that one cannot be content with one-electron Dirac theory, and one must rely upon QED, even for building a mean-field (one-body) theory. Since QED is a many-body theory in which the number of particles is not conserved, one ought to work in Fock space in order to build properly the state vectors, the Hamiltonian and the energy functional to be minimised. To begin with and to fix the notation, we briefly summarise the standard Dirac and Fock descriptions of electrons and positrons in QED (Bjorken and Drell 1965, Itzykson and Zuber 1980).

2.1. Bare electron/positron Fock states

Let us consider a basis of bispinor eigenfunctions of the Dirac Hamiltonian $h_D \equiv \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m$. Each function of this basis is characterised by a set 'k' of quantum numbers corresponding to operators that commute with h_D (for instance momentum and polarisation, or radial and angular momenta). For each value of the quantum numbers k, h_D has a positive eigenvalue ω_k and a negative eigenvalue $-\omega_k$, with the corresponding eigenfunctions $u_{xk} \equiv u_k(\boldsymbol{x})$ and $v_{xk} \equiv v_k(\boldsymbol{x})$:

$$\begin{aligned} h_D u_k(\boldsymbol{x}) &= \omega_k u_k(\boldsymbol{x}) \\ h_D v_k(\boldsymbol{x}) &= -\omega_k v_k(\boldsymbol{x}). \end{aligned} \tag{2.1}$$

The bispinor operator-valued electron–positron field $\Psi_x = \Psi(x)$ can be expanded on the eigenbasis, with operator components b and d^+:

$$\Psi_x = \sum_k (u_{xk} b_k + v_{xk} d_k^+). \tag{2.2}$$

This expansion can be considered as a particular rotation in Fock space, and we therefore introduce the following shorthand matrix notations. The field Ψ and the eigenfunctions u_k and v_k are bispinors, which may be written as four-component columns:

$$U \equiv (u|0) \qquad V \equiv (0|v) \qquad R \equiv U + V = (u|v). \tag{2.3}$$

The orthogonality and completeness of the eigenbasis are expressed by $R^+R = 1$ and $RR^+ = 1$ respectively, and (2.2) becomes

$$(\Psi) = (u|v)\begin{pmatrix} b \\ d^+ \end{pmatrix} = R\begin{pmatrix} b \\ d^+ \end{pmatrix} \tag{2.4}$$

where indices and summations are understood. Because of the unitarity of R, the canonical anticommutation rules for Ψ can be written in terms of b and d as

$$\{b_k, b_q^+\} = \{d_k, d_q^+\} = \delta_{kq} \tag{2.5}$$

and all other anticommutators vanish. As usual the b's and d's are interpreted as *bare electron* and *bare positron* destruction operators, respectively, and their Hermitian conjugates as *bare electron* and *bare positron* creation operators. We denote $|0\rangle$ and call the *bare vacuum* the Fock state characterised by

$$b_k|0\rangle = d_k|0\rangle = 0 \qquad \text{for every } k.$$

The Fock space is then spanned by $|0\rangle$ and by the excitations resulting from the action of the b^+'s and d^+'s on $|0\rangle$. Fock states can be characterised by the expectation values of operators like for instance the electron and positron numbers N^e and N^p, the charge Q, or the kinetic energy (or free Hamiltonian) H_D, defined as

$$N_k^e \equiv b_k^+ b_k \qquad N^e \equiv \sum_k N_k^e \tag{2.6}$$

$$N_k^p \equiv d_k^+ d_k \qquad N^p \equiv \sum_k N_k^p \tag{2.7}$$

$$Q \equiv e(N^p - N^e) \tag{2.8}$$

$$H_D \equiv \sum_k \omega_k (N_k^e + N_k^p) \tag{2.9}$$

respectively. Because of the commutation relations (2.5), one has

$$[Q, b_k^+] = -eb_k^+ \qquad [Q, d_k^+] = +ed_k^+ \tag{2.10}$$

$$[H_D, b_k^+] = \omega_k b_k^+ \qquad [H, d_k^+] = \omega_k d_k^+ \tag{2.11}$$

and one says that b_k^+ creates a charge $-e$ and an energy ω_k, and that d_k^+ creates a charge $+e$ and an energy ω_k. It is of interest for the following discussion to note that, in this framework, the distinction between electrons and positrons is based on the sign of their charge and not on the sign of their energy: the one-particle Dirac theory has been 'reinterpreted' in (2.2) by considering the components d^+ of Ψ upon negative eigenvalue eigenstates v as creation operators, while the components b upon positive eigenvalue eigenstates u are considered as destruction operators. Positrons as well as electrons have a positive kinetic energy, and the bare vacuum $|0\rangle$ is the Fock state with minimum H_D expectation value.

2.2. Vacuum subtraction and normal ordering

It is manifest from equations (2.6) to (2.9) that the operators N^e, N^p, Q and H_D have vanishing expectation values in the bare vacuum $|0\rangle$: electric charge and kinetic energy are measured relative to the bare vacuum. Subtracting from a one-body operator, its vacuum expectation value is equivalent to setting it into normal order, that is to permuting the bare creation and destruction operators as if they anticommuted, until all the creation operators have moved towards the left-hand side. This ordering operation, denoted $\mathcal{N}[\ldots]$, is defined relative to the bare vacuum and particles, and we refer to it as the *bare normal ordering.* One has for instance

$$Q = -e\left(\int \mathrm{d}\boldsymbol{x}(\Psi_x^+ \,.\, \Psi_x) - \langle 0| \int \mathrm{d}\boldsymbol{x}\,(\Psi_x^+ \,.\, \Psi_x)|0\rangle\right) = -e\mathcal{N}\left[\int \mathrm{d}\boldsymbol{x}\,(\Psi_x^+ \,.\, \Psi_x)\right] \tag{2.12}$$

$$H_D = \int \mathrm{d}\boldsymbol{x}\,(\Psi_x^+ h_D \Psi_x) - \langle 0| \int \mathrm{d}\boldsymbol{x}\,(\Psi_x^+ h_D \Psi_x)|0\rangle = \mathcal{N}\left[\int \mathrm{d}\boldsymbol{x}\,(\Psi_x^+ h_D \Psi_x)\right] \tag{2.13}$$

where it is again manifest that the bare vacuum has zero charge and zero kinetic energy. Since (2.12) allows us to consider $Q(\boldsymbol{x}) = -e\mathcal{N}[\Psi_x^+ \,.\, \Psi_x]$ as the local charge density operator, a Hamiltonian for electrons in a local external potential $\Omega(\boldsymbol{x})$ reads

$$H_D + \int \mathrm{d}\boldsymbol{x}\,\Omega(\boldsymbol{x})Q(\boldsymbol{x}) = \mathcal{N}\left[\int \Psi_x^+(h_D - e\Omega(\boldsymbol{x}))\Psi_x\right]. \tag{2.14}$$

It is normally ordered and therefore has a vanishing expectation value in the bare vacuum: the energy is still measured relative to the bare vacuum. Of course this does not mean that the bare vacuum remains the Fock state of minimum energy: the Fock state describing the true vacuum can be different from the bare vacuum state $|0\rangle$.

3. Bogoliubov transformation with charge conservation

We now proceed with building a variational ansatz in Fock space. Since the Hamiltonian of QED conserves electric charge but does not conserve particle number, we consider an ansatz of definite electric charge without imposing a definite number of particles. We build the ansatz as a Slater determinant of quasiparticles of definite charge: the dressed particles. These dressed particles have the same electric charges as the bare particles, and the distinction between dressed electrons and dressed positrons is made non-ambiguously according to their charge, not according to their energy. It is worth mentioning that in contrast with one-particle Dirac theory, there is no negative energy continuum in QED.

3.1. Dressed particles and dressed vacuum

To build quasiparticles, we need to introduce a new set of operators $\tilde{b}$ and $\tilde{d}$ that satisfy the same canonical anticommutation relations (2.5) as those for b and d, and that bear the same respective charges:

$$\{\tilde{b}_n, \tilde{b}_m^+\} = \{\tilde{d}_n, \tilde{d}_m^+\} = \delta_{nm} \tag{3.1}$$

$$[Q, \tilde{b}_n^+] = -e\tilde{b}_n^+ \qquad [Q, \tilde{d}_n^+] = +e\tilde{d}_n^+. \tag{3.2}$$

This can be achieved using a linear transformation which mixes the b's with the d^+'s (and the b^+'s with the d's):

$$\begin{pmatrix} \tilde{b}_n \\ \tilde{d}_n^+ \end{pmatrix} \equiv T_{nk} \begin{pmatrix} b_k \\ d_k^+ \end{pmatrix} \equiv \begin{pmatrix} c_{nk} & s_{nk} \\ \sigma_{nk} & \kappa_{nk} \end{pmatrix} \begin{pmatrix} b_k \\ d_k^+ \end{pmatrix} \tag{3.3}$$

where the summation over k is understood and where the transformation T is unitary:

$$T^+T = 1 \qquad TT^+ = 1. \tag{3.4}$$

Although the transformation (3.3) is not the more general way to fulfil (3.1) and (3.2), we adopt it because it allows one to recover the standard DF theory as an approximation and offers interesting new features to be discussed below.

Because of (3.1), one can again interpret the new operators $\tilde{b}$ and $\tilde{d}$ as destruction operators. We shall call *dressed electrons* and *dressed positrons* the corresponding particles, and denote $|\tilde{0}\rangle$ the corresponding *dressed vacuum.* The charge of this vacuum is zero since the transformation (3.3) conserves electric charge, but in general its energy is different from that of the bare vacuum $|0\rangle$. One can analyse the content of $|\tilde{0}\rangle$ in terms of bare particles: $|\tilde{0}\rangle$ is a linear combination of the bare vacuum with one-pair states $b^+d^+|\tilde{0}\rangle$, two-pair states, etc. The expectation values of the numbers of electrons and positrons in $|\tilde{0}\rangle$ are equal:

$$\langle\tilde{0}|N^{\mathrm{P}}|\tilde{0}\rangle = \langle\tilde{0}|N^{\mathrm{e}}|\tilde{0}\rangle = \mathrm{Tr}(ss^+) = \mathrm{Tr}(\sigma\sigma^+). \tag{3.5}$$

One can now express the electron-positron field in terms of the transformed creation-destruction operators. Using (2.4) and (3.3) one gets

$$(\Psi) = \tilde{R}\begin{pmatrix} \tilde{b} \\ \tilde{d}^+ \end{pmatrix} \tag{3.6}$$

with

$$\tilde{R} \equiv RT^+. \tag{3.7}$$

Like in (2.3), one can write

$$\tilde{U} \equiv (\tilde{u}|0) \qquad \tilde{V} \equiv (0|\tilde{v}) \qquad \tilde{R} = \tilde{U} + \tilde{V} = (\tilde{u}|\tilde{v}) \tag{3.8}$$

where the $\tilde{u}$'s and $\tilde{v}$'s correspond to the dressed electrons $\tilde{b}$ and dressed positrons $\tilde{d}^+$, respectively. The unitarity of $\tilde{R}$ expresses that the vectors $\tilde{u}$ and $\tilde{v}$ form a new orthonormal basis in the space of bispinor wavefunctions. Note that $\tilde{R}$ contains the same information as does the transformation T itself: physical quantities may be expressed in terms of T or $\tilde{R}$, depending on convenience.

3.2. Bogoliubov transformation

Electrons and positrons do not appear in a symmetrical manner in the expansions (2.4) or (3.6). In order to make explicit the electron-positron symmetry and to obtain a more manageable formulation, it is useful, though not necessary, to double these equations. We write the expansions of Ψ and Ψ^+, and we gather under the same notation B the destruction operators b and d. B^+ creates a bare particle, electron or positron, and $\tilde{B}^+$ creates a dressed particle. We then have in matrix notation

$$\left(\begin{array}{c} \Psi \\ \hline \Psi^+ \end{array}\right) = \left(\begin{array}{c|c} U & V \\ \hline V^* & U^* \end{array}\right)\left(\begin{array}{c} B \\ \hline B^+ \end{array}\right) = \left(\begin{array}{c|c} \tilde{U} & \tilde{V} \\ \hline \tilde{V}^* & \tilde{U}^* \end{array}\right)\left(\begin{array}{c} \tilde{B} \\ \hline \tilde{B}^+ \end{array}\right) \tag{3.9}$$

and, in the same way, (3.3) becomes

$$\begin{pmatrix} \tilde{B} \\ \tilde{B}^+ \end{pmatrix} = \left(\begin{array}{cc|cc} c & 0 & 0 & s \\ 0 & \kappa^* & \sigma^* & 0 \\ \hline 0 & s^* & c^* & 0 \\ \sigma & 0 & 0 & \kappa \end{array}\right) \begin{pmatrix} B \\ B^+ \end{pmatrix} \tag{3.10}$$

The transformations (3.9) and (3.10) are formally of the same kind as the *Bogoliubov transformations* used in statistical and nuclear physics, where they are useful to describe superconductivity or superfluidity. We shall therefore refer to them as (charge-conserving) Bogoliubov transformations. Although the dynamics and interpretations may be different in the various fields of physics—for instance the first equality in (3.9) expresses the reinterpretation of Dirac theory rather than pairing phenomena—we now have at our disposal the machinery of Bogoliubov theory.

3.3. General Bogoliubov ansatz for an atom

We can now build on $|\tilde{0}\rangle$ a charged state $|\tilde{\Phi}\rangle$ having a definite number of dressed particles:

$$|\tilde{\Phi}\rangle \equiv \prod_n \tilde{B}_n^+ |\tilde{0}\rangle. \tag{3.11}$$

$|\tilde{\Phi}\rangle$ is an independent dressed particle state characterised by the set of quantum numbers n appearing in (3.11), or equivalently by the occupation number matrix

$$\tau_{mn} \equiv \langle \tilde{\Phi} | \tilde{B}_n^+ \tilde{B}_m | \tilde{\Phi} \rangle. \tag{3.12}$$

In the study of an atom, the dressed particles will be electrons and the index n will denote the atomic levels. The matrix τ is diagonal and made up with ones and zeros: it may be split into a dressed electron part $\tau^{\mathrm{e}}_{mn} \equiv \langle \tilde{\Phi} | \tilde{b}_n^+ \tilde{b}_m | \tilde{\Phi} \rangle$ and a dressed positron part $\tau^{\mathrm{p}}_{mn} \equiv \langle \tilde{\Phi} | \tilde{d}_n^+ \tilde{d}_m | \tilde{\Phi} \rangle$, and expressed as

$$\tau = \begin{pmatrix} \tau^{\mathrm{e}} & 0 \\ 0 & \tau^{\mathrm{p}} \end{pmatrix}. \tag{3.13}$$

We also introduce the following matrix $\tilde{\tau}$ for later convenience:

$$\tilde{\tau} \equiv \begin{pmatrix} \tau^{\mathrm{e}} & 0 \\ 0 & -\tau^{\mathrm{p}} \end{pmatrix}. \tag{3.14}$$

Here, τ^{p} describes the occupation of dressed positron states in the system under study. The minimisation of energy in an atom will automatically lead to $\tau^{\mathrm{p}} = 0$ because of the repulsive potential felt by the positrons. This is in contrast with the usual arbitrary practice consisting of leaving empty the positron-like states of DF theory.

3.4. Charge-violating Bogoliubov transformation

Instead of T (3.3), one might have considered a more general linear transformation mixing all the b, b^+, d and d^+ operators. For such a general charge-violating transformation, the double notation (3.9) is necessary, and the matrix in (3.10) is no longer half-full of zeros. This more general transformation leads to a charged vacuum, to particles of indefinite charge and finally to an ansatz of indefinite charge. Then one should constrain the electric charge of the variational ansatz in expectation value only,

via a Lagrange multiplier. Such a procedure may be useful for instance to describe electron-electron pairing phenomena in a relativistic theory of superconductivity, which is outside the scope of this paper. To close this remark, we stress that, in our formalism, the charge is manifestly invariant under the Bogoliubov transformation, and the variational states are eigenstates of the charge operator.

3.5. Densities and reordering relations

One-particle operators are generally expressed in terms of normally ordered products of fields. It is therefore useful to introduce the density operator, defined as the normally ordered tensor product $\mathcal{N}[\Psi^+ \otimes \Psi]$. If we gather under the same notations i, j, k, l, the position (or the momentum) *and* the component indices running from 1 to 4, the expectation value D of the density operator in a given Fock state $|\Phi\rangle$ is

$$D_{ji} \equiv \langle \Phi | \mathcal{N}[\Psi_i^+ \Psi_j] | \Phi \rangle. \tag{3.15}$$

In particular, the bare vacuum density vanishes, and with (3.9)

$$\tilde{\rho}_{ji} \equiv \langle \tilde{0} | \mathcal{N}[\Psi_i^+ \Psi_j] | \tilde{0} \rangle = \langle \tilde{0} | \Psi_i^+ \Psi_j | \tilde{0} \rangle - \langle 0 | \Psi_i^+ \Psi_j | 0 \rangle = (\tilde{V}\tilde{V}^+ - VV^+)_{ji}. \tag{3.16}$$

The dressed vacuum density $\tilde{\rho}$ is the difference between two projection operators $\tilde{V}\tilde{V}^+$ and VV^+. The operator VV^+, which projects upon the negative eigenvalue eigenstates v of the free Dirac Hamiltonian $h_D = \boldsymbol{\alpha}.\boldsymbol{p} + \beta m$, characterises the Dirac sea of 'negative energy states'. $\tilde{V}\tilde{V}^+$ projects upon the $\tilde{v}$'s, and characterises the 'dressed Dirac sea'. $\tilde{\rho}$ characterises the difference between the bare vacuum $|0\rangle$ and the dressed Bogoliubov vacuum $|\tilde{0}\rangle$, and we refer to $\tilde{\rho}$ as the *vacuum polarisation density*. The expectation value of any one-body operator in the Bogoliubov vacuum $|\tilde{0}\rangle$ may be written in terms of $\tilde{\rho}$. For instance, the local electric charge density of the Bogoliubov vacuum at point $\boldsymbol{x}$ is $-e$ times the vacuum density $\tilde{\rho}$ taken at point $\boldsymbol{x}$ and traced over the component indices.

Since the Bogoliubov ansatz (3.11) is given in terms of the dressed vacuum $|\tilde{0}\rangle$ and of the dressed particle operators $\tilde{B}$, it is useful to introduce the normal ordering $\tilde{\mathcal{N}}$ corresponding to $|\tilde{0}\rangle$, where we bring now the $\tilde{B}$'s to the right-hand side and the $\tilde{B}^+$'s to the left-hand side. Then, one has the reordering relations

$$\mathcal{N}[\Psi_i^+ \Psi_j] = \tilde{\mathcal{N}}[\Psi_i^+ \Psi_j] + \tilde{\rho}_{ji} \tag{3.17}$$

$$\begin{aligned} \mathcal{N}[\Psi_i^+ \Psi_j^+ \Psi_l \Psi_k] = {} & \tilde{\mathcal{N}}[\Psi_i^+ \Psi_j^+ \Psi_l \Psi_k] + \tilde{\rho}_{ki} \tilde{\mathcal{N}}[\Psi_j^+ \Psi_l] \\ & + \tilde{\rho}_{lj} \tilde{\mathcal{N}}[\Psi_i^+ \Psi_k] - \tilde{\rho}_{li} \tilde{\mathcal{N}}[\Psi_j^+ \Psi_k] - \tilde{\rho}_{kj} \tilde{\mathcal{N}}[\Psi_i^+ \Psi_l] + \tilde{\rho}_{ki}\tilde{\rho}_{lj} - \tilde{\rho}_{li}\tilde{\rho}_{kj}. \end{aligned} \tag{3.18}$$

As can be seen, reordering a one-body operator introduces a c-number (the vacuum polarisation $\tilde{\rho}$), and reordering a two-body operator introduces both a c-number and a one-body operator. The reordering relation (3.17) and the expansion (3.9) allow us to write the density matrix of the Bogoliubov ansatz (3.11) in terms of the occupation matrix $\tilde{\tau}$ (3.14):

$$\tilde{D}_{ji} \equiv \langle \tilde{\Phi} | \mathcal{N}[\Psi_i^+ \Psi_j] | \tilde{\Phi} \rangle = \tilde{R}\tilde{\tau}\tilde{R}^+ + \tilde{\rho}. \tag{3.19}$$

The first term of the right-hand side of (3.19) describes the occupied dressed particle states of the system, for instance the dressed electron states in an atom. One notes that the dressed electron and positron densities appear with a relative minus sign in $\tilde{\tau}$ (3.14) corresponding to charge conjugation. The second term is the non-trivial contribution $\tilde{\rho}$ of the dressed vacuum.

4. Minimisation equations

Now, we search for the ground state of a given Hamiltonian in a sector of the Fock space characterised by a given electric charge. In the specific case of atomic physics, the electric charge is $-e$ times the considered atomic number, and the Hamiltonian is built from Coulomb-gauge QED in the complete Fock space of nuclear, electronic and electromagnetic degrees of freedom. From a variational point of view, one restricts the variational space to tensor products of a nuclear, a photon and an electron-positron state. In practice the nuclear state is frozen, and the photons are excluded. This leads to an electron-positron Hamiltonian, which is the sum of a kinetic energy term, an external potential generated by the nucleus and the two-body Coulomb interaction.

Note that there are other ways of selecting an electron-positron sector in the Fock space of QED. For instance, one may begin by performing a suitable unitary transformation in the Fock space in order to uncouple the photons from the electrons and positrons up to a given order in the coupling constant (Cohen-Tannoudji *et al* 1987–88, Schwinger 1948). Then one may exclude the photons of the variational space. Although the elimination of photons generally results in a many-body electron-positron Hamiltonian, and although the formalism developed below is still relevant to such cases, we shall restrict ourselves to one-body and two-body interactions. Two different problems of relativistic atomic physics overlap here. The first one is the building of a Fock-space Hamiltonian for electrons and positrons, for instance via the Schwinger transformation; and the second one is the building of the corresponding mean-field approximation. Of course in this paper we focus on the second point.

The minimisation method amounts to approximating the ground state of a system by the state of minimum energy (i.e. Hamiltonian expectation value) in a given variational space. The approximate ground-state energy necessarily lies higher than the exact one, and the larger the variational space, the lower the minimum energy and the better the approximation. Here, the variational Fock state $|\tilde{\Phi}\rangle$ is characterised by the Bogoliubov transformation T (3.3) and the set of occupation numbers τ (3.12). We first choose a given τ, thus fixing the respective numbers of dressed electrons and dressed positrons that we want to consider. Then, we introduce the *Bogoliubov-Dirac-Fock* (BDF) variational space, that is the set of $|\tilde{\Phi}\rangle$'s (3.11), for the Bogoliubov transformation T taking all its possible values under the constraint of unitarity. Since we only consider charge-conserving Bogoliubov transformations, all the $|\tilde{\Phi}\rangle$ states in this BDF variational space have the same electric charge. Next one minimises the energy in the BDF variational space. Following the usual procedure, we search for stationary points of the energy, among which the minimum must be determined.

4.1. The Bogoliubov energy and the vacuum polarisation

In the following we consider a Hamiltonian of the general form

$$H \equiv \mathcal{N}[h_{ij}\Psi_i^+\Psi_j + \mathcal{V}_{ijkl}\Psi_i^+\Psi_j^+\Psi_l\Psi_k] \tag{4.1}$$

where the summation over repeated indices is understood, h is the one-body Hamiltonian and $\mathcal{V}$ is an antisymmetric two-body interaction

$$\mathcal{V}_{ijkl} = \mathcal{V}_{klij} = -\mathcal{V}_{ijlk}. \tag{4.2}$$

Because of the normal ordering, the energy of the bare vacuum is equal to zero, thus offering a reference for all other energies. With the help of the reordering relations

(3.17) and (3.18), it is straightforward to reorder the Hamiltonian (4.1) on the variational dressed vacuum $|\tilde{0}\rangle$. One finds

$$H = \tilde{E}_0 + (h + \tilde{\Gamma})_{ij} \tilde{\mathcal{N}}[\Psi_i^+ \Psi_j] + \mathcal{V}_{ijkl} \tilde{\mathcal{N}}[\Psi_i^+ \Psi_j^+ \Psi_l \Psi_k] \tag{4.3}$$

where we have introduced the following notations and definitions:

$$\tilde{\Gamma}_{ij} \equiv 4 \mathcal{V}_{likj} \tilde{\rho}_{kl} \equiv \text{vacuum polarisation potential} \tag{4.4}$$

and

$$\tilde{E}_0 \equiv \langle \tilde{0} | H | \tilde{0} \rangle = \mathrm{Tr}(h + \tfrac{1}{2}\tilde{\Gamma})\tilde{\rho} \equiv \text{dressed vacuum energy.} \tag{4.5}$$

It is important to note that the reordering yields a c-number shift $\tilde{E}_0$ and a one-body potential $\tilde{\Gamma}$. The c-number, one-body and two-body terms in (4.3) depend on the Bogoliubov rotation (3.3): different Bogoliubov rotations lead to different normal orderings $\tilde{\mathcal{N}}$, and therefore to different splittings of the same Hamiltonian into c-number, one-body and two-body contributions. Although the functional form $\mathcal{V}$ of the two-body interaction remains unchanged (it would have been changed if we had taken into account three-body interactions), the residual two-body interaction in Fock space $\mathcal{V}_{ijkl} \tilde{\mathcal{N}}[\Psi_i^+ \Psi_j^+ \Psi_l \Psi_k]$ has definitely been modified since the normal ordering $\tilde{\mathcal{N}}$ is different from $\mathcal{N}$. For a given Bogoliubov rotation, one could discard the vacuum energy $\tilde{E}_0$ on the usual ground that it is a c-number. This is what one does when, instead of using (2.1) and (2.2), one decides to develop the electron-positron field Ψ upon an eigenbasis of a given reference Hamiltonian $h_D + \Omega_{\mathrm{ref}}$, which is Furry's bound interaction picture (Furry 1951, Jauch and Rohrlich 1976). However, if one wants to compare the effects of different Bogoliubov transformations, one must keep $\tilde{E}_0$. Despite the fact that one cannot measure the vacuum energy in an absolute manner, one can compare the energies of different dressed vacuum states $|\tilde{0}\rangle$, the reference energy being the energy of the bare vacuum $|0\rangle$. Moreover, the dressed vacuum energy will contribute to the total energy of a system in the state $|\tilde{\Phi}\rangle$ (3.11), and in principle it will be necessary to take it into account to compare the energies of different Bogoliubov states, especially in a variational procedure.

The expectation values in the Bogoliubov state $|\tilde{\Phi}\rangle$ (3.11) of normally ordered products of fields are

$$\langle \tilde{\Phi} | \tilde{\mathcal{N}}[\Psi_i^+ \Psi_j] | \tilde{\Phi} \rangle = \langle \tilde{\Phi} | \tilde{\mathcal{N}}[(\tilde{V}^* \tilde{B} + \tilde{U}^* \tilde{B}^+)_i (\tilde{U} \tilde{B} + \tilde{V} \tilde{B}^+)_j] | \tilde{\Phi} \rangle = (\tilde{R} \tilde{\tau} \tilde{R}^+)_{ji} \tag{4.6}$$

and in a similar manner

$$\langle \tilde{\Phi} | \tilde{\mathcal{N}}[\Psi_i^+ \Psi_j^+ \Psi_l \Psi_k] | \tilde{\Phi} \rangle = (\tilde{R} \tilde{\tau} \tilde{R}^+)_{lj} (\tilde{R} \tilde{\tau} \tilde{R}^+)_{ki} - (\tilde{R} \tilde{\tau} \tilde{R}^+)_{kj} (\tilde{R} \tilde{\tau} \tilde{R}^+)_{li}. \tag{4.7}$$

The expectation value of H in the state $|\tilde{\Phi}\rangle$ is then readily obtained from (4.3) as

$$\tilde{E} = \tilde{E}_0 + \mathrm{Tr}(h + \tilde{\Gamma} + \tfrac{1}{2}\Gamma)(\tilde{R} \tilde{\tau} \tilde{R}^+) \tag{4.8}$$

where we introduced the *screening potential*

$$\Gamma_{ij} \equiv 4 \mathcal{V}_{likj} (\tilde{R} \tilde{\tau} \tilde{R}^+)_{kl} \tag{4.9}$$

interpreted as the mean potential that is felt by one dressed particle under the influence of the others. The energy of the Bogoliubov state is the sum of two contributions: the dressed vacuum energy $\tilde{E}_0$ and the second term of (4.8), which corresponds to the dressed particle cloud characterised by $\tilde{R} \tilde{\tau} \tilde{R}^+$. The vacuum polarisation results not only in an energy $\tilde{E}_0$ but also in an extra one-body potential $\tilde{\Gamma}$ that appears here as a correction to the external potential Ω already present in h, and to the usual screening potential Γ.

4.2. The Bogoliubov-Dirac-Fock (BDF) equations

The stationarity equations cannot be derived in the same way as in usual non-relativistic HF theory, since we deal here with densities (3.19) that do not satisfy any idempotence relation (i.e. $\tilde{D}^2 \neq \tilde{D}$). However, the stationarity of the Bogoliubov energy (4.8) as a functional of the unitary transformation $\tilde{R}$ leads to

$$[\tilde{h}, \tilde{R}\tilde{\tau}\tilde{R}^+ + \tilde{V}\tilde{V}^+] = 0 \qquad \tilde{h} \equiv h + \Gamma + \tilde{\Gamma}. \tag{4.10}$$

We will refer to (4.10) as the BDF equations, and to $\tilde{h}$ as the BDF (mean-field) Hamiltonian. These equations look very much like the standard HF or DF equations (Ring and Schuck 1980, Kim 1967). However, the BDF equations have essential new features. First, the dressed electrons and the dressed positrons appear via the matrix $\tilde{\tau}$ (3.14) with opposite signs, which corresponds to their opposite electric charges. Secondly, besides the usual screening term Γ, the BDF Hamiltonian $\tilde{h}$ contains the vacuum polarisation term $\tilde{\Gamma}$ originating from the non-perturbative modification of the vacuum as due to the external field and to the other charged particles. Finally the polarised vacuum contributes the amount $\tilde{E}_0$ (4.5) to the total BDF energy. We will consider in more detail the relationship between the BDF and the standard DF theories in the following section. However, it is now and henceforth clear that the BDF equations reduce to the DF equations if the following three conditions are fulfilled: (i) the system under study contains no dressed positrons, (ii) one neglects the effects of the vacuum polarisation potential on the electrons of the system, and (iii) finally one neglects the energy of the polarised vacuum.

The BDF equations (4.10) have a structure similar to that of the usual HF or DF equations. Therefore, at least in principle, they may be solved by the same numerical methods, involving calculations in position space leading to a system of coupled integro-differential equations, or simultaneous diagonalisation of the BDF Hamiltonian and the density, both approximated in a finite-dimensional space. However, some practical differences are expected. The main one lies in the calculation of the self-consistent Hamiltonian, which involves the vacuum density (3.16). For instance, in an iterative diagonalisation procedure one should proceed through the following steps. Begin with a given first iteration bispinor basis $(\tilde{u}, \tilde{v})$ corresponding to a first iteration matrix $\tilde{R}$, and build the matrix $\tilde{R}\tilde{\tau}\tilde{R}^+ + \tilde{V}\tilde{V}^+$; then build the BDF Hamiltonian

$$\tilde{h}_{ij} = h_{ij} + 4\mathscr{V}_{likj}(\tilde{R}\tilde{\tau}\tilde{R}^+ + \tilde{V}\tilde{V}^+ - VV^+)_{kl}$$

diagonalise it and build the second iteration basis $(\tilde{u}, \tilde{v})$ with its eigenvectors; and iterate the procedure until convergence is achieved.

Like in HF theory, solving the stationarity BDF equation (4.10) is not sufficient to determine completely the minimum energy state. In HF calculations, the occupation matrix is filled in a way that minimises the HF energy for a given number of occupied levels. Although the total HF energy is *not* the sum of the energies of the occupied levels, this usually leads to filling the lowest HF levels. Here in BDF theory, the occupation numbers must be chosen in a way that minimises the total BDF energy for a given total charge. This prescription offers the possibility of adding a dressed pair to the system, in accordance with the arbitrariness of the splitting of the eigenstates of the BDF Hamiltonian into the electron-like $\tilde{u}$'s on the one hand and the positron-like $\tilde{v}$'s on the other. Another difference with HF theory is that the BDF one-particle states are built upon a polarised vacuum, the energy of which must in principle be taken into account.

4.3. BDF Hamiltonian for the Dirac-Coulomb problem

As an example, here we make the notations explicit for the problem of electrons in a local potential $\Omega(\boldsymbol{x})$, with a scalar two-body interaction. The corresponding Hamiltonian is of the form

$$H = \mathcal{N}\left[\int \mathrm{d}\boldsymbol{x}\, \Psi_x^+(h_\mathrm{D}+\Omega)\Psi_x + \int \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y}\, \mathcal{V}(\boldsymbol{x}-\boldsymbol{y})(\Psi_x^+ . \Psi_x)(\Psi_y^+ . \Psi_y)\right]. \tag{4.11}$$

This is a particular case of (4.1), where each of the indices i, j, k, l stands for a position $\boldsymbol{x}, y, z, t$ and a component index α, β, g, δ. The Dirac Hamiltonian and the external potential are

$$(h_\mathrm{D}+\Omega)\begin{pmatrix} \boldsymbol{xy} \\ \alpha\beta \end{pmatrix} = \begin{pmatrix} [m+\Omega(x)]\langle \boldsymbol{x}|\boldsymbol{y}\rangle & \langle \boldsymbol{x}|\boldsymbol{\sigma} . \boldsymbol{p}|\boldsymbol{y}\rangle \\ \langle \boldsymbol{x}|\boldsymbol{\sigma} . \boldsymbol{p}|\boldsymbol{y}\rangle & [-m+\Omega(x)]\langle \boldsymbol{x}|\boldsymbol{y}\rangle \end{pmatrix}_{\alpha\beta} \tag{4.12}$$

where m is the electron-positron mass, σ the Pauli matrices and $\boldsymbol{p}$ the momentum operator. The antisymmetrical two-body interaction is

$$\mathcal{V}\begin{pmatrix} \boldsymbol{xyzt} \\ \alpha\beta\gamma\delta \end{pmatrix} = \frac{1}{2}\,\mathcal{V}(\boldsymbol{x}-\boldsymbol{y})[\delta(\boldsymbol{x}-\boldsymbol{z})\delta(\boldsymbol{y}-\boldsymbol{t})\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta(\boldsymbol{x}-\boldsymbol{t})\delta(\boldsymbol{y}-\boldsymbol{z})\delta_{\alpha\delta}\delta_{\beta\gamma}]. \tag{4.13}$$

The resulting screening potential Γ (4.9) is the sum of a local direct term Γ^D and a non-local exchange term Γ^E (summation over repeated indices is assumed):

$$\Gamma^\mathrm{D}\begin{pmatrix} \boldsymbol{xy} \\ \alpha\beta \end{pmatrix} = 2\delta(\boldsymbol{x}-\boldsymbol{y})\delta_{\alpha\beta}\mathcal{V}(\boldsymbol{x}-\boldsymbol{z})(\tilde{R}\tilde{\tau}\tilde{R}^+)\begin{pmatrix} \boldsymbol{zz} \\ \gamma\gamma \end{pmatrix} \tag{4.14}$$

and

$$\Gamma^\mathrm{E}\begin{pmatrix} \boldsymbol{xy} \\ \alpha\beta \end{pmatrix} = -2\mathcal{V}(\boldsymbol{x}-\boldsymbol{y})(\tilde{R}\tilde{\tau}\tilde{R}^+)\begin{pmatrix} \boldsymbol{xy} \\ \alpha\beta \end{pmatrix}. \tag{4.15}$$

The density appearing in Γ^D is taken at a single point z, and traced over γ; it is the dressed particle charge density at point z (note that dressed electrons and dressed positrons appear with a relative minus sign in $\tilde{\tau}$). In the same way the vacuum polarisation potential (4.4) is the sum of a direct term $\tilde{\Gamma}^\mathrm{D}$ and an exchange term $\tilde{\Gamma}^\mathrm{E}$:

$$\tilde{\Gamma}^\mathrm{D}\begin{pmatrix} \boldsymbol{xy} \\ \alpha\beta \end{pmatrix} = 2\delta(\boldsymbol{x}-\boldsymbol{y})\delta_{\alpha\beta}\mathcal{V}(\boldsymbol{x}-\boldsymbol{z})\tilde{\rho}\begin{pmatrix} \boldsymbol{zz} \\ \gamma\gamma \end{pmatrix} \tag{4.16}$$

$$\tilde{\Gamma}^\mathrm{E}\begin{pmatrix} \boldsymbol{xy} \\ \alpha\beta \end{pmatrix} = -2\mathcal{V}(\boldsymbol{x}-\boldsymbol{y})\tilde{\rho}\begin{pmatrix} \boldsymbol{xy} \\ \alpha\beta \end{pmatrix}. \tag{4.17}$$

The density $\tilde{\rho}$ in $\tilde{\Gamma}^\mathrm{D}$ is taken at point z and traced over the component index γ: it is the local charge density of the Bogoliubov vacuum. Since we only considered charge-conserving Bogoliubov transformations (3.3), the total charge of the vacuum (i.e. $\tilde{\rho}$ traced over γ and z) vanishes. However the charge density at a given point z in general does not vanish, and contributes to the total mean field. Finally, (4.16) and (4.17) are new terms arising from the BDF derivation of the relativistic mean-field theory. Note that, unlike perturbative corrections accounting for vacuum or radiative effects in standard DF calculations, these terms are to be included in the iteration procedure since they appear in the self-consistent equations of mean-field theory.

5. Connection with the usual Dirac–Fock theory

The standard DF theory is generally derived without any reference to Fock space (Kim 1967): a system of N electrons is described by an N-electron wavefunction, and the Hamiltonian acts in the space of N-electron wavefunctions (configuration space). The DF variational space is the space of N-particle bispinor wavefunctions of the form

$$\phi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) = \mathscr{A}\phi_1(\boldsymbol{x}_1) \ldots \phi_N(\boldsymbol{x}_N) \tag{5.1}$$

where $\mathscr{A}$ means antisymmetrisation. This standard procedure ignores the reinterpretation of the negative eigenvalue eigenstates of the Dirac Hamiltonian. However, it can still be expressed in the language of second quantisation, as follows. One considers negative energy electrons rather than positrons, and all the operators appearing in the expansion (2.2) of the Dirac field are considered as destruction operators:

$$\Psi_x = \sum_k (u_{kx}\beta_{k+} + v_{kx}\beta_{k-}) \tag{5.2a}$$

with

$$\beta_{k+} \equiv b_k \qquad \beta_{k-} \equiv d_k^+ \tag{5.2b}$$

where the index $\pm$ refers to the sign of the corresponding Dirac eigenvalue. The vacuum corresponding to the expansion (5.2), defined by $\beta_{k+}|V\rangle = \beta_{k-}|V\rangle = 0$, is the vacuum of the local operator Ψ_x. The standard DF rotation mixes the $\beta_{k\pm}$ operators to build one-particle operators $\tilde{\beta}_i$ corresponding to the one-particle wavefunctions ϕ_i appearing in (5.1). Also, the variational space of the N-particle wavefunctions ϕ (5.1) is equivalent to the variational space of the Fock states $|\tilde{\Phi}_{\mathrm{DF}}\rangle \equiv \tilde{\beta}_1^+ \ldots \tilde{\beta}_N^+|V\rangle$. The stationarity equations are derived in exactly the same formal way as in non-relativistic HF theory, thus leading to the DF equations. These are only stationarity equations, and one does not look for a minimum of the DF 'energy' functional since it is not bounded below. Instead one has to consider that 'negative energy states are of no physical interest' (Kim 1967) for the study of bound electron states, and therefore should not be considered in the occupation-number matrix.

The relationship between this point of view on the one hand, and the BDF point of view on the other, is as follows. Because of (5.2b), the DF rotation mixing the $\beta_\pm$'s is identical to the Bogoliubov transformation (3.3) mixing the b's and the d^+'s. Therefore, the DF and BDF variational spaces are in one-to-one correspondence. However, according to Dirac's reinterpretation, the bare vacuum $|0\rangle$ of QED is the sea of 'negative energy states', i.e. $|0\rangle = (\Pi\beta_-^+)|V\rangle$, or equivalently $|V\rangle \equiv (\Pi d^+)|0\rangle$. Since $|0\rangle$ is the reference for the calculation of energies (normal ordering), the energy $E_v \equiv \langle V|H|V\rangle$ of the DF vacuum $|V\rangle$ is infinite. The Bogoliubov rotation among the destruction operators β, or equivalently between the b's and d^+'s does not change the vacuum $|V\rangle$, whereas it does change the vacuum $|0\rangle$ into a dressed vacuum $|\tilde{0}\rangle$. Now the Fock state describing the physical vacuum is $|\tilde{0}\rangle$ rather than $|V\rangle$, and the Fock state describing the atom is $|\tilde{\Phi}_{\mathrm{BDF}}\rangle \equiv \tilde{b}_1^+ \ldots \tilde{b}_N^+|\tilde{0}\rangle$ rather than $|\tilde{\Phi}_{\mathrm{DF}}\rangle \equiv \tilde{\beta}_1^+ \ldots \tilde{\beta}_N^+|V\rangle$. The DF vacuum $|V\rangle$ contributes the infinite energy $E_v \equiv \langle V|H|V\rangle$ to the energy of the DF Fock state $|\tilde{\Phi}_{\mathrm{DF}}\rangle$; it is common practice to remove this infinite energy in order to recover the standard DF energy. However, doing so is rather arbitrary and leaves aside the polarisation terms arising from the dressed vacuum $|\tilde{0}\rangle$. These contributions can be viewed as resulting from the quasi-cancellation of infinite energies corresponding to the successive emptying of the bare Dirac sea, and filling of the dressed Dirac sea.

Indeed, the dressed vacuum $|\tilde{0}\rangle$ is the Bogoliubov transform of $|0\rangle = (\Pi d)|V\rangle$, where $|V\rangle$ is invariant under the Bogoliubov transformation. It may therefore be written

$$|\tilde{0}\rangle = \Pi \tilde{d}|V\rangle = (\Pi \tilde{d})(\Pi d^+)|0\rangle = (\Pi \tilde{\beta}_-^+)(\Pi \beta_-)|0\rangle.$$

The main difference between the DF and BDF methods is that the respective variational Fock states are not built upon the same vacua. The vacuum $|V\rangle$ of DF theory lies in the middle of the spectrum with an energy E_v, and this is why the DF state is only a stationary point of the DF energy, not a minimum. Furthermore, within the standard DF point of view, one does not know *a priori* which DF states must be considered as electrons or positrons, except in the non-relativistic limit. In this case, the energy gap around the vacuum is large, and one can clearly distinguish between electron-like (positive eigenvalue) states $\tilde{\beta}_+$ and positron-like (negative eigenvalue) states $\tilde{\beta}_-$. It is precisely in this limit that the BDF vacuum effects are small, and that the BDF equations (4.10) reduce to the usual DF equations. However, even in this case, the standard point of view does not indicate why one should not fill the DF 'negative energy states' for the minimisation of the total energy. There is no such ambiguity in the BDF point of view. Since in an atom the central potential is attractive for electrons and repulsive for positrons, it will be energetically unfavourable to add dressed positrons to the system. Dressed positrons will not appear in the density matrix, not because of a supplementary condition, but as a natural result of the minimisation of the BDF energy.

5.1. The 'no-pair' approximation

Previous attempts to build the DF theory upon QED have led to DF-like theories with modified mean-field Hamiltonians, for instance 'positive energy projected Hamiltonians' resulting from the 'no-pair' theory of Sucher (Reinhard *et al* 1971) that we discuss below. The electron-positron field, appearing in the Fock-space Hamiltonian (4.1) and expanded over the free Dirac waves in (2.2), can be separated into an electron destruction term Ψ_e and a positron creation term Ψ_p^+:

$$\Psi = \Psi_e + \Psi_p^+ \tag{5.3}$$

with

$$\Psi_e \equiv \sum_k u_k b_k \qquad \Psi_p^+ \equiv \sum_k v_k d_k^+.$$

The Fock-space Hamiltonian (4.1) can therefore be split into a sum of terms involving Ψ_e and Ψ_p. One can gather under the name H_{pair} the terms that involve pair operators of the form $\Psi_e^+\Psi_p^+$ or $\Psi_e\Psi_p$; the remaining terms are pure scattering terms involving no pair operators and can be gathered under the name $H_{\text{no-pair}}$. Then

$$H = H_{\text{no-pair}} + H_{\text{pair}}. \tag{5.4}$$

The idea underlying the no-pair theory is to employ a variational procedure to treat $H_{\text{no-pair}}$, and a perturbative procedure to take H_{pair} into account (Sucher 1983). Since $H_{\text{no-pair}}$ conserves the respective numbers of electrons and positrons, it is possible to consider variational Fock states with no positrons and with a definite number N of electrons. As a result, the positron part of the no-pair Hamiltonian does not contribute to the energy, and one can keep the electron part $H^e_{\text{no-pair}}$ only:

$$\begin{aligned} H^e_{\text{no-pair}} &\equiv \mathcal{N}[h_{ij}\Psi^+_{ei}\Psi_{ej} + \mathcal{V}_{ijkl}\Psi^+_{ei}\Psi^+_{ej}\Psi_{el}\Psi_{ek}] \\ &= (u^+_{ki}h_{ij}u_{jp})b^+_p b_k + (u^+_{ki}u^+_{pj}\mathcal{V}_{ijlm}u_{lq}u_{mr})b^+_k b^+_p b_q b_r \end{aligned} \tag{5.5}$$

where the indices i, j, l and m stand for the position and the bispinor component index, and where k, p, q, r stand for the quantum numbers characterising the free Dirac waves. Then, the energy for a Slater determinant characterised by the electronic no-pair density $\rho^{e}_{\text{no-pair}} \equiv \langle b^{+} b \rangle$ is (indices and summations are understood)

$$E^{e}_{\text{no-pair}} = (u^{+} h u)\rho^{e}_{\text{no-pair}} + 2(u^{+} u^{+} \mathcal{V} u u)\rho^{e}_{\text{no-pair}} \rho^{e}_{\text{no-pair}} \tag{5.6}$$

and the corresponding mean-field Hamiltonian is

$$\begin{aligned} h^{e}_{\text{no-pair}} &\equiv \partial E^{e}_{\text{no-pair}} / \partial \rho^{e}_{\text{no-pair}} \\ &= (u^{+} h u) + 4(u^{+} u^{+} \mathcal{V} u u)\rho^{e}_{\text{no-pair}}. \end{aligned} \tag{5.7}$$

The same mean-field Hamiltonian (5.7) may be derived from the stationarity equations in the space of N-electron wavefunctions of the form (5.1), if one uses the positive energy projected configuration-space Hamiltonian

$$h_{\text{proj}} = \Lambda^{+}_{a}(h_{\text{D}a} + \Omega_{a})\Lambda^{+}_{a} + \Lambda^{+}_{a}\Lambda^{+}_{b}(\mathcal{V}_{ab})\Lambda^{+}_{a}\Lambda^{+}_{b} \tag{5.8}$$

where the indices a and b numbering the electrons are summed over, and where Λ_a stands for the projection operator

$$\Lambda^{+}(\boldsymbol{x}_a, \boldsymbol{y}_a) \equiv \sum_{k} u_k(\boldsymbol{x}_a) u^{+}_{k}(\boldsymbol{y}_a). \tag{5.9}$$

As long as it excludes the positron states from the variational space, such a 'positive energy projected' theory suffers neither from variational collapse nor from continuum dissolution. However, it does not lead to the same results as the standard DF theory since the projection operators Λ^{+} alter the mean-field Hamiltonian. The effects of the projection may be compensated by the corrections due to H_{pair}, which must be supposed to be small in order to be evaluated via a perturbative expansion.

Now we show how the no-pair theory can be considered as a restriction of the BDF theory. In the BDF theory, the pair effects result from the mixing (3.3) of electron destruction operators b with positron creation operators d^{+}. This mixing is characterised by the off-diagonal blocks s and σ of the Bogoliubov transformation T (3.3). If we restrict ourselves to $s = \sigma = 0$, then we get a smaller variational space, for which $|\tilde{0}\rangle = |0\rangle$, $\tilde{\rho} = 0$ and $\tilde{\Gamma} = 0$. With this restriction, we do not take into account vacuum polarisation, and the particles are not dressed: one may call this approximation the 'bare' approximation. In the restricted variational space under consideration, the variational state (3.11) reduces to

$$|\Phi\rangle \equiv \Pi(c^{*} b^{+})\Pi(\kappa d^{+})|0\rangle \tag{5.10}$$

where the diagonal blocks c and κ of the Bogoliubov transformation (3.3) are both unitary. The energy (4.8) then becomes

$$\tilde{E} = h_{ij}(\tilde{R}\tilde{\tau}\tilde{R}^{+})_{ji} + 2\mathcal{V}_{likj}(\tilde{R}\tilde{\tau}\tilde{R}^{+})_{kl}(\tilde{R}\tilde{\tau}\tilde{R}^{+})_{ji}. \tag{5.11}$$

$\tilde{E}$ cannot be varied as before because now we impose supplementary conditions on $\tilde{R}$: the functions $\tilde{u}$ are linear combinations of the u's but not of the v's, and vice versa. However, with (3.7) and (2.3), one can rewrite the densities as

$$\tilde{R}\tilde{\tau}\tilde{R}^{+} = (U + V)(T^{+}\tilde{\tau}T)(U + V)^{+} \tag{5.12}$$

where $T^{+}\tilde{\tau}T$ has the form

$$T^{+}\tilde{\tau}T = \begin{pmatrix} c^{+}\tau^{\text{e}}c & 0 \\ 0 & -\kappa^{+}\tau^{\text{p}}\kappa \end{pmatrix} \equiv \begin{pmatrix} \rho^{\text{e}} & 0 \\ 0 & -\rho^{\text{p}} \end{pmatrix}. \tag{5.13}$$

Because of this block-diagonal structure expressing the non-appearance of pairs, the density can be split into an electron part and a positron part:

$$\tilde{R}\tilde{\tau}\tilde{R}^{+} = U(T^{+}\tilde{\tau}T)U^{+} + V(T^{+}\tilde{\tau}T)V^{+}.$$

The matrices U and U^{+} appearing in the first term pick up only the electron density ρ^{e}, and the matrices V and V^{+} appearing in the second one pick up only the positron density ρ^{p}. In the same way, the energy $\tilde{E}$ (5.11) can be split into an electron energy $\tilde{E}^{e}$, a positron energy $\tilde{E}^{p}$ and a crossed energy $\tilde{E}^{ep}$, with

$$\begin{aligned}
&\tilde{E} = \tilde{E}^{e} + \tilde{E}^{p} + \tilde{E}^{ep} \\
&\tilde{E}^{e} \equiv h_{ij}(UT^{+}\tilde{\tau}TU^{+})_{ji} + 2\mathcal{V}_{likj}(UT^{+}\tilde{\tau}TU^{+})_{kl}(UT^{+}\tilde{\tau}TU^{+})_{ji} \\
&\tilde{E}^{p} \equiv h_{ij}(VT^{+}\tilde{\tau}TV^{+})_{ji} + 2\mathcal{V}_{likj}(VT^{+}\tilde{\tau}TV^{+})_{kl}(VT^{+}\tilde{\tau}TV^{+})_{ji} \\
&\tilde{E}^{ep} \equiv 4\mathcal{V}_{likj}(UT^{+}\tilde{\tau}TU^{+})_{kl}(VT^{+}\tilde{\tau}TV^{+})_{ji}.
\end{aligned} \tag{5.14}$$

In the trivial case, where the external potential Ω and the two-body interaction $\mathcal{V}$ are switched off, one can see that the positrons as well as the electrons give a positive contribution to $\tilde{E}$ since, by construction, $U^{+}h_{D}U$ is positive and $V^{+}h_{D}V$ is negative. Now, with $\Omega \neq 0$ and $\mathcal{V} \neq 0$, $\rho^{e} = c^{+}\tau^{e}c$ and $\rho^{p} = \kappa^{+}\tau^{p}\kappa$ are density matrices in the usual sense of HF theory, and the stationarity equations for $\tilde{E}$ under the normalisation constraints $\rho^{e}\rho^{e} = \rho^{e}$ and $\rho^{p}\rho^{p} = \rho^{p}$ are derived in the standard way, leading to

$$[\rho^{e}, \tilde{h}^{e}] = 0 \qquad \text{and} \qquad [\rho^{p}, \tilde{h}^{p}] = 0 \tag{5.15}$$

with the electron and positron mean-field Hamiltonians

$$\tilde{h}^{e} \equiv (u^{+}hu) + 4(u^{+}u^{+}\mathcal{V}uu)\rho^{e} - 4(v^{+}u^{+}\mathcal{V}vu)\rho^{p} \tag{5.16}$$

$$\tilde{h}^{p} \equiv -(v^{+}hv) + 4(v^{+}v^{+}\mathcal{V}vv)\rho^{p} - 4(u^{+}v^{+}\mathcal{V}uv)\rho^{e} \tag{5.17}$$

respectively. If one considers a system involving no positrons, for instance when calculating the structure of an atom within the bare approximation, ρ^{p} vanishes and the electron mean-field Hamiltonian (5.16) reduces to $h^{e}_{\text{no-pair}}$ given by (5.7). The no-pair approximation can therefore be considered as a restriction of the variational BDF approximation. This different manner of considering the no-pair approximation, that is its derivation from QED via a minimisation principle, leads to a different way of improving it: if the no-pair approximation is viewed as resulting from a truncation of the Fock-space Hamiltonian, the effects of the truncated part H_{pair} will be evaluated via perturbation methods, but on the other hand if it is viewed as resulting from a narrowing of the variational space, it appears as a restriction of the more general BDF variational theory that should be able to describe pair effects even in non-perturbative situations.

5.2. The no-pair approximation in Furry's picture

In the framework of no-pair theory, there is some arbitrariness in splitting the Hamiltonian into pair and no-pair components. The splitting (5.3) relies on the expansion (2.2) over the free Dirac waves, and is therefore related to the free Dirac Hamiltonian h_{D}. The no-pair Hamiltonian conserves the number of *bare* particles, and this leads to the appearance in the configuration-space Hamiltonian of projection operators Λ^{+} over the eigenstates of the *free Dirac Hamiltonian* h_{D}. However, following Furry (1951), one may expand the electron-positron field Ψ over the eigenstates of a reference

Hamiltonian $h_F = h_D + \Omega_F$, Ω_F being a given one-body potential. If Ω_F is not too large, there is still a gap between the positive and negative eigenvalues of h_F. Then, one can split Ψ into a positive eigenvalue part Ψ_{eF} and a negative eigenvalue part Ψ^+_{pF} as follows:

$$\Psi = \Psi_{eF} + \Psi^+_{pF} \tag{5.18}$$

with

$$\Psi_{eF} \equiv \sum_n u_{nF} b_{nF}$$

$$\Psi^+_{pF} = \sum_n v_{nF} d^+_{nF}$$

and

$$h_F u_{nF} = \varepsilon_n u_{nF} \qquad \varepsilon_n > 0$$

$$h_F v_{nF} = \eta_n v_{nF} \qquad \eta_n < 0.$$

Neglecting the problem of ordering, one may then split the Fock-space Hamiltonian into the pair and no-pair Hamiltonians corresponding to the definitions of Ψ_{eF} and Ψ_{pF} (Sucher 1983):

$$H = H^F_{\text{no-pair}} + H^F_{\text{pair}}. \tag{5.19}$$

The splittings (5.3) and (5.4) described in the previous subsection are recovered for $\Omega_F = 0$, but one can also choose Ω_F equal to the external potential, or any Ω_F supposed to be suitable for the problem at hand, as long as it allows a clear distinction between the corresponding electron-like and positron-like states. Different choices for the reference potential Ω_F lead to different splittings of the Fock-space Hamiltonian, to different mean-field Hamiltonians and to different configuration-space Hamiltonians. Λ will be replaced in (5.8) and (5.9) by the operator projecting upon the positive eigenvalue eigenstates of the reference Hamiltonian h_F.

This procedure can also be recovered via BDF theory, although with an important new feature: because of the two-body interaction, the one-body potential is modified in Furry's picture. Indeed, in the BDF approach we started from the Fock-space Hamiltonian (4.1) ordered on the bare vacuum $|0\rangle$. The electron and positron operators b_{nF} and d_{nF} defined in Furry's picture differ from the bare electron and positron operators b_k and d_k, and therefore their vacuum $|0_F\rangle$ differs from the bare vacuum $|0\rangle$. $|0_F\rangle$ and $|0\rangle$ are related by the Bogoliubov transformation, which diagonalises the reference Hamiltonian h_F. The Fock-space Hamiltonian (4.1) is independent of the representation, but it may be reordered on Furry's vacuum:

$$H = \tilde{E}_F + (h + \tilde{\Gamma}_F)_{ij} \mathcal{N}_F[\Psi^+_i \Psi_j] + \mathcal{V}_{ijkl} \mathcal{N}_F[\Psi^+_i \Psi^+_j \Psi_l \Psi_k]. \tag{5.20}$$

This procedure introduces the energy $\tilde{E}_F$ of Furry's vacuum $|0_F\rangle$, as well as a polarisation potential $\tilde{\Gamma}_F$ arising from the two-body interaction. As long as the reference potential Ω_F determining Furry's representation is given once and for all, the fixed c-number $\tilde{E}_F$ can be ignored since it corresponds to a mere shift of the zero of energies. This is not the case for the polarisation potential $\tilde{\Gamma}_F$, which modifies the one-body interaction. Therefore the Furry representation introduces an extra one-body potential $\tilde{\Gamma}_F$, which should be taken into account in the no-pair Hamiltonian $H^F_{\text{no-pair}}$ deduced from (5.20). The interpretation of this term is straightforward: by construction, the no-pair theory

in the Furry representation does not take into account the effects of Furry's electron-positron pairs $b_F^+ d_F^+ |0_F\rangle$. However, the electron operators b_F, the positron operators d_F and the vacuum $|0_F\rangle$ are dressed by bare electron-positron pairs as indicated in § 3, and $\tilde{\Gamma}_F$ arises as the consequence of these bare electron-positron pairs.

Furthermore, one may note that the total one-body potential depends upon the reference Hamiltonian h_F because of the two-body interaction. Here, we have a two-body interaction because we started from QED in Coulomb gauge (the gauge invariance has been lost because of the elimination of the photons from the variational space), and the situation is different if one considers the covariantly quantised version of QED: then there is no two-body interaction and Furry's picture can be used without modifying the one-body potentials.

5.3. The 'optimised' Furry picture

In the previous subsection we have adopted a reference Hamiltonian once and for all, and set apart the corresponding no-pair term of the Hamiltonian of QED (Sucher 1980). One can also consider an optimisation of this procedure. Mittleman (1981) has carried out the minimisation of the energy as a functional of the reference potential Ω_F, and concluded that the optimum Ω_F is the Dirac-Fock potential. This leads to replacing the projection operators Λ^+ appearing in the configuration-space Hamiltonian (5.8) by self-consistent projection operators upon the positive eigenvalue eigenstates of the mean-field Hamiltonian itself. The practical consequence is that it is useless to write these projection operators explicitly, thus recovering the standard DF procedure. However, the derivation of this result leaves aside the vacuum contributions to the energy. Changing Ω_F implies altering the energy $\tilde{E}_F$ of the Furry vacuum. $\tilde{E}_F$ is a c-number, and is of no importance if the vacuum is defined once and for all. However, $\tilde{E}_F$ should be taken into account if one wants to vary it. Of course this is what the Bogoliubov transformation is designed for. The BDF method is a natural way to render stationary the energy, taking self-consistently into account what is called electron, positron and vacuum.

5.4. The DF equations as an 'unpolarised vacuum' approximation

The polarisation terms occurring in the BDF equations arise from the modifications of the vacuum under the influence of the external potential and of the dressed electron-positron density. These terms are certainly small in a great number of physical situations, especially if the external potential is small. Then, at least as a first step, one may neglect these vacuum polarisation terms. In this approximation the BDF Hamiltonian (4.10) reduces to the DF Hamiltonian:

$$\tilde{h} \simeq h + \Gamma. \tag{5.21}$$

If there is no positron in the system under study, one has to diagonalise $\tilde{h}$ and fill only the electron part τ^e of the occupation-number matrix τ (3.13); this is equivalent to the standard DF procedure. It is worth noting that, since this '$\tilde{\Gamma} \simeq 0$' approximation is not a narrowing of the variational space but a truncation of the mean-field Hamiltonian, the DF theory is not rigorously variational. Because of this breakdown of the minimisation procedure, the standard DF method may not be applied in situations where non-perturbative vacuum polarisation effects take place.

6. Finite-basis approximation from the BDF point of view

In the non-relativistic HF theory, the variational state is a Slater determinant of normalised one-particle wavefunctions. A method often used for solving the HF equations is the finite-basis approximation. In this approximation one imposes that the one-particle wavefunctions belong to a given finite-dimensional vector space, with the consequence that the HF problem reduces to a non-linear matrix problem. Furthermore, the considered finite-dimensional linear space may depend on one or several 'non-linear' parameters. Since the non-relativistic Schrödinger kinetic energy $-\Delta/2m$ is positive, with the consequence that the HF Hamiltonian is bounded below, the HF energy approaches the ground-state energy from above, and one can improve the approximation by minimising the HF energy as a function of these non-linear parameters.

This procedure has been transposed to treat the standard DF equations (Kim 1967, Stanton and Havriliak 1984, Quiney *et al* 1987). Then the variational N-electron wavefunctions are Slater determinants of N normalised one-particle bispinor wavefunctions taken within a given finite-dimensional space. For instance, the most common procedure consists of expanding the 'large' and 'small' components of the wavefunctions on a two Pauli-spinor basis. However, in the relativistic context specific difficulties arise because the spectrum of the Dirac operator $h_D = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m$ describing the kinetic energy has a negative continuum. Indeed, though the Fock-space Hamiltonian H (4.1) and the energy functional $\tilde{E}$ (4.8) *are* bounded below, the mean-field Hamiltonian $\tilde{h} = h_D + \Gamma + \tilde{\Gamma}$ occurring in the stationarity equations (4.10) *is not* bounded below. As a consequence, the eigenvalues of a finite-basis approximation of the BDF Hamiltonian are not necessarily upper bounds of the exact eigenvalues of the BDF Hamiltonian, and they do not necessarily converge towards these exact eigenvalues as the size of the basis is increased. Some eigenvalues can decrease indefinitely when one tries to optimise the finite-basis parameters (variational collapse), and unphysical eigenvalues (spurious states) can appear among sensible eigenvalues (Gazdy and Ladanyi 1984). Moreover, the spurious states cannot merely be ignored, even when they are unequivocally identified, since they may spoil the wavefunctions corresponding to the correctly approximated part of the spectrum. In fact, one can overcome these difficulties, and avoid the 'finite-basis disease' (Kutzelnigg 1984, Grant 1986, Goldman and Dalgarno 1986, Quiney *et al* 1987, Johnson *et al* 1988). With these methods, one still deals with the standard DF equations and Hamiltonian, but one looks for stationary points of the DF energy, not for minima. Provided that *ad hoc* conditions are imposed on the basis sets (correct non-relativistic limit and correct boundary conditions), the finite-basis method allows one to solve the DF equations with a high degree of accuracy (Wilson 1989).

Just like the DF Hamiltonian, the BDF Hamiltonian is not bounded below, and the same treatment should be prescribed. However, we propose an alternative point of view on the finite-basis method, focusing on its physical meaning rather than on numerical efficiency. Remaining within the minimisation process in Fock space as described in the previous sections, one can work with the bounded-below Fock-space Hamiltonian, and make the finite-basis approximation *at the Fock-space level.* We then consider the BDF mean-field approximation of a 'finite-basis quantum-field theory', rather than the finite-basis approximation of a mean-field theory.

In this section we are mainly interested in the finite-basis aspects, which are present even if there is no two-body interaction ($\mathcal{V} = 0$). Therefore, and for the sake of

simplicity, we consider a one-body Hamiltonian only: $H = \mathcal{N}[\Psi^+ h \Psi]$. Starting from the u's and v's described in § 2, one can build a basis of the space of bispinor wavefunctions with the following successive rotations ($R^+R = RR^+ = -S^+S = SS^+ = 1$, and $c_n^2 + s_n^2 = 1$):

$$\begin{cases} u_k \\ v_k \end{cases} \rightarrow \begin{cases} u_n \equiv u_k R^+_{kn} \\ v_n \equiv v_k S^+_{kn} \end{cases} \rightarrow \begin{cases} \phi_n \equiv c_n u_n + s_n v_n \\ \xi_n \equiv s_n u_n + c_n v_n. \end{cases} \tag{6.1a}$$

The corresponding creation–destruction operators are

$$\begin{cases} b_k \\ d_k^+ \end{cases} \rightarrow \begin{cases} b_n \equiv R_{nk} b_k \\ d_n^+ \equiv S_{nk} d_k^+ \end{cases} \rightarrow \begin{cases} \beta_n \equiv c_n b_n + s_n d_n^+ \\ \delta_n^+ \equiv -s_n b_n + c_n d_n^+ \end{cases} \tag{6.1b}$$

and the corresponding expansions of Ψ are

$$\Psi = \sum_k (u_k b_k + v_k d_k^+) = \sum_n (u_n b_n + v_n d_n^+) = \sum_n (\phi_n \beta_n + \xi_n \delta_n^+). \tag{6.2}$$

The first rotation (characterised by R and S) does not change the vacuum since $b_n|0\rangle = d_n|0\rangle = 0$, but the second one (characterised by c and s) does. We denote $|0'\rangle$ and call *basis vacuum* the Fock state characterised by $\beta_n|0'\rangle = \delta_n|0'\rangle = 0$, for every n. The rotations (6.1) are particular Bogoliubov transformations, and one can reorder the Hamiltonian:

$$H = \mathcal{N}[\Psi^+ h \Psi] = E'_0 + \mathcal{N}'[\Psi^+ h \Psi] \tag{6.3}$$

where $\mathcal{N}'$ is the normal ordering corresponding to $|0'\rangle$, and where E'_0 is the energy of $|0'\rangle$. We refer to E'_0 as the *basis energy*. It is a c-number depending on the basis

$$E'_0 = \sum_n [s_n^2 (u_n^+ h u_n - v_n^+ h v_n) - s_n c_n (v_n^+ h u_n + u_n^+ h v_n)]. \tag{6.4}$$

The Hamiltonian is now expressed in terms of ϕ_n and ξ_n. One can introduce a finite-basis approximation in the following way. The Fock space is spanned by $|0'\rangle$ and the excitations created by the actions of the β_n^+'s and the δ_n^+'s. Let us consider a finite set B of indices, and let us call $\mathcal{F}_B$ the finite-dimensional subspace of Fock space spanned by $|0'\rangle$ and the excitations created by the β_n^+ and δ_n^+ for $n \in B$. The restriction of Ψ to $\mathcal{F}_B$ is

$$\psi_B = \sum_{n \in B} (\phi_n \beta_n + \xi_n \delta_n^+). \tag{6.5}$$

If, in a variational procedure, the variational states are restricted to $\mathcal{F}_B$, the expectation values of H (6.3) are

$$\langle H \rangle = E'_0 + \langle \mathcal{N}'[\Psi^+ h \Psi] \rangle = E'_0 + \langle \mathcal{N}'[\Psi_B^+ h \Psi_B] \rangle. \tag{6.6}$$

The problem then reduces to the treatment of the restricted Hamiltonian $H_B \equiv \mathcal{N}'[\Psi_B^+ h \Psi_B]$, and to the calculation of the basis energy E'_0. The restricted Hamiltonian H_B, which still has the standard normally ordered form (4.1), can be treated by the BDF method described in § 4. In the absence of two-body interaction, this reduces to the diagonalisation of the matrix of h in the finite basis $(\phi_n, \xi_n)_{n \in B}$:

$$(h_B)_{nm} \equiv \begin{pmatrix} \phi_n^+ h \phi_m & \phi_n^+ h \xi_m \\ \xi_n^+ h \phi_m & \xi_n^+ h \xi_m \end{pmatrix}. \tag{6.7}$$

The basis energy E'_0 (6.4) is the sum of terms labelled by $n \in B$, and of terms labelled by $n \notin B$ corresponding to the part of the basis that is not used to describe the system.

The optimisation of the basis leads, in particular, to minimising these 'off-restricted-basis' terms. If the external potential is negligible *out of* the region covered by the restricted basis, the vacuum will be significantly polarised only *in* this region, and it will be a good approximation to choose $s_n = 0$ for $n \notin B$. The basis energy then reduces to a finite sum

$$E'_0 = \sum_{n \in B} [s_n^2(u_n^+ h u_n - v_n^+ h v_n) - s_n c_n (v_n^+ h u_n + u_n^+ h v_n)]. \tag{6.8}$$

One must note that the one-particle energies will not be the mere eigenvalues of h_B. In the relativistic case, important new features appear. The calculation of the one-particle energies will involve (i) the basis energy E'_0 (6.8) originating from the choice of the basis, (ii) a BDF vacuum energy $\tilde{E}_0$ originating from the dynamical polarisation of the vacuum in the finite basis (it is here a finite trace over $n \in B$) and (iii) the eigenvalues of the BDF Hamiltonian (6.7) (counted positively or negatively, since the BDF density involves a matrix $\tilde{\tau}$ with eigenvalues ± 1). Note that this procedure allows an optimisation of the basis by minimisation of energy, according to the Rayleigh-Ritz principle. There is no such optimisation possible in DF calculations.

In the usual finite-basis methods, the upper and lower components of the bispinor wavefunctions are expanded separately on an upper-component basis and a lower-component basis. This amounts to considering bispinor basis functions with either a vanishing small component or a vanishing large component. Although it can be used for an efficient numerical expansion of the solutions of the DF equations, such a basis does not have a clear physical status. Indeed, such a basis can be obtained by a rotation from the free bispinor waves u and v, but this leads to an infinite basis energy E'_0. More physically sensible basis sets may be built using (6.1), leading to a finite or vanishing basis energy. Since the calculations involved in this procedure are more complicated than the standard finite-basis calculations, due to the vacuum contribution and to the form of the considered basis functions, they should not be used for solving problems for which the standard DF approach is successful. However, these calculations are manageable and worthwhile, if not necessary, for special situations out of the domain of validity of the standard DF theory (systems in very strong external fields).

7. Conclusions

In this work we have shown how QED can provide stable foundations for a relativistic mean-field theory of electrons and positrons in an external field. Despite the fact that the Dirac Hamiltonian $\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m$ is unbounded below, a minimisation method can be elaborated like in the non-relativistic theory by consistently taking into account the normal ordering of the Fock operators, and the Dirac interpretation of negative spectra. This leads to modifications of the well known Dirac-Fock equations. The relativistic character of the underlying theory—namely QED—appears in a natural way via a vacuum energy and vacuum polarisation terms. These terms do not arise from QED via perturbation theory, but are determined in a self-consistent manner during the minimisation procedure.

Since it incorporates from the beginning the ideas of Dirac reinterpretation, this formalism allows a sensible interpretation of the mean-field equations (for instance *negative* eigenvalues of the self-consistent Hamiltonian correspond to *positive* energies, as expected). The minimisation of the energy functional can be carried out without

any ambiguity, even when bound electronic states lie very deep in the mass gap. This is not the case when dealing with the usual DF theory, since this theory does not take positron states into account.

The approach developed in this paper leads to vacuum polarisation terms, which are necessary for the internal consistency of the relativistic mean-field theory, and which should therefore be taken into account in proper self-consistent calculations, independently of the magnitude of the physical effects. These new variational vacuum polarisation terms are expected to be numerically small in usual situations, and may then be neglected or used to derive perturbative corrections similar to those commonly taken into account. However, in the very relativistic regime, for instance in the vicinity of very high-Z nuclei, they may become larger, and then one expects results different from those of perturbative calculations. We think that in such extreme cases, vacuum polarisation effects will have to be taken self-consistently into account for the theory to be meaningful. The non-perturbative vacuum polarisation may therefore play a role in the understanding of QED in very strong external fields.

The standard DF equations as well as the different kinds of projected DF equations appeared as particular restrictions or approximations of the formalism.

As an illustration we have considered electrons in an external potential, the two-body interaction being swiched off ($\alpha = 0$). We obtained a new insight into the 'finite-basis methods' and we described a different manner to introduce finite-basis relativistic calculations.

The main assumption underlying this work is that the electron-positron Hamiltonian is bounded below in Fock space. However, although the kinetic energy operator in Fock space is positive due to Dirac reinterpretation, the existence of a ground state for the total electron-positron Hamiltonian depends on the interactions. The influence of the two-body interaction on the variational stability will be considered in the following paper.

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