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From quantum electrodynamics to mean-field theory: II. Variational stability of the vacuum of quantum electrodynamics in the mean-field approximation

P Chaix†, D Iracane† and P L Lions‡

† Commissariat à l'Energie Atomique, Centre d'Etudes de Bruyères-le-Châtel, Service PTN, BP 12, 91680, Bruyères-le-Châtel, France

‡ Université Paris-Dauphine, Ceremade, Place de Lattre de Tassigny, 75775 Paris Cedex 16, France

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Abstract. We use a minimisation principle to analyse the variational stability of the translationally invariant vacuum of quantum electrodynamics, with a Coulomb two-body interaction. We show how the magnitude of the coupling constant α determines the existence of a stable variational ground state. This ground state does exist within the considered variational space, provided that α is smaller than a critical value α_c. The ground state collapses if α is larger than α_c. Bounds on the critical value α_c are given, and the physical value $\alpha = 1/137$ is shown to be undercritical.

1. Introduction

The Dirac-Fock (DF) theory has led to calculations of impressive accuracy and to numerous successes in the study of atomic and molecular structures (Grant 1970, Lindgren and Rosen 1974, Quiney *et al* 1987, Gorceix *et al* 1987). However, this theory presents features that make its interpretation and implementation delicate, leading for example to continuum dissolution (Brown and Ravenhall 1951, Sucher 1985), to variational collapse (Wallmeier and Kutzelnigg 1981, Schwarz and Wallmeier 1982, Stanton and Havriliak 1984) and to the appearance of spurious states in finite-basis calculations unless specific constraints are imposed on the basis sets (Grant 1986). These difficulties all originate from the fact that the free Dirac Hamiltonian $h_D = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m$ describing the kinetic energy is not bounded below. That is to say that DF theory does not take into account Dirac's reinterpretation of the vacuum. This reinterpretation, which is most naturally expressed in the language of second quantisation, leads to quantum electrodynamics (QED) and to a positive kinetic energy Hamiltonian in Fock space. Consequently, a minimisation procedure in Fock space does not suffer from the same difficulties as a minimisation in the space of bispinor wavefunctions. Such a procedure allows one to establish the relativistic mean-field theory upon QED via a minimisation principle, as was developed in the previous paper (Chaix and Iracane 1989, hereafter referred to as I). The stationarity equations associated with this formalism are very similar to standard DF equations, but include additional terms that are interpreted as describing vacuum polarisation effects. However, the boundedness of the complete Fock-space Hamiltonian *including interactions* will in general

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depend on the interactions that are considered. It is therefore necessary, for a minimisation procedure to make sense, that the interactions do not spoil the boundedness of the electron-positron Fock-space Hamiltonian.

The interaction terms that may be added to the kinetic energy to form the total electron-positron Hamiltonian are of two kinds: there is the one-body interaction, or external potential, resulting from given charged sources, and there is the interaction between electrons and positrons. In Coulomb-gauge QED, electrons and positrons interact via the instantaneous Coulomb two-body interaction and via the exchange of photons. In this paper, like in I, we consider the minimisation problem within a variational subspace of Fock space that contains no photon, so that the electron-positron interaction reduces to the Coulomb contribution.

Since the study of the vacuum is the necessary first step for building more complicated states describing charged systems, in the present work we focus our attention on this point. Depending upon the form and intensity of the interactions, three situations can happen: (i) the bare vacuum is stable and remains the lowest energy state; (ii) the bare vacuum is unstable, and the lowest energy state is a non-trivial Fock state; and (iii) the bare vacuum is unstable, the energy has no minimum and the theory 'collapses'. This collapse does not arise from the 'negative energy states' of the Dirac Hamiltonian since there are no longer negative kinetic energies in QED, but is due to the interactions. As a first step, we consider the effects of the Coulomb two-body interaction on vacuum stability, no one-body external potential being applied. The question that arises is whether the bare vacuum $|0\rangle$ is the lowest energy translationally invariant uncharged state in Fock space.

We discuss this issue by means of the 'Bogoliubov-Dirac-Fock' (BDF) variational method described in I, and wonder whether or not the bare vacuum $|0\rangle$ is the lowest energy translationally invariant uncharged state *within the BDF variational space.* Therefore, the work presented in this paper is a variational study of the vacuum of QED from a non-perturbative point of view, and a first illustration of the specific aspects of BDF mean-field theory.

We proceed through the following steps. First we describe the momentum-diagonal Bogoliubov rotation in Fock space, which allows one to define the variational dresssed BDF vacuum. Then we explicitly give the energy of the dressed vacuum and the BDF mean-field Hamiltonian as functionals of the Bogoliubov angles. As described in I, the BDF stationarity equations for the energy involve this BDF Hamiltonian and the vacuum density. We cast these equations in the form of a set of two coupled integral equations, the gap equations. Finally, for the specific case of the Coulomb two-body interaction, we carry on the explicit study of the minimum BDF energy and show under which conditions on the coupling constant α the minimisation problem has a solution.

2. The BDF Hamiltonian and the variational BDF energy

The physical system under study, that is the vacuum, is assumed to be translationally invariant. Therefore, we only consider translationally invariant variational BDF states and momentum-diagonal Bogoliubov transformations. It must be noted that allowing non-translationally invariant BDF variational states may enable us to lower the energy, due to the non-linearity of the BDF equations; however a study of this possible spontaneous symmetry breaking is beyond the scope of the present paper.

The momentum representation is of course best suited to state the problem, and we begin by rewriting in this representation the main quantities that appear in the formalism. The kinetic Dirac Hamiltonian is momentum-diagonal and, for a given momentum $\boldsymbol{k}$,

$$h_{\mathrm{D}}(\boldsymbol{k}) \equiv \boldsymbol{\alpha}\cdot\boldsymbol{k} + \beta m = \begin{pmatrix} m & (\boldsymbol{\sigma}\cdot\boldsymbol{k}) \\ (\boldsymbol{\sigma}\cdot\boldsymbol{k}) & -m \end{pmatrix} \tag{1}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices. $h_{\mathrm{D}}(\boldsymbol{k})$ can be diagonalised and its eigenvalues are $\pm\omega_k$:

$$R^{+}(\boldsymbol{k})h_{\mathrm{D}}(\boldsymbol{k})R(\boldsymbol{k}) = \begin{pmatrix} \omega_k & 0 \\ 0 & -\omega_k \end{pmatrix}$$

$$R(\boldsymbol{k}) = \begin{pmatrix} c_k & -s_k(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}}) \\ s_k(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}}) & c_k \end{pmatrix} \qquad \hat{\boldsymbol{k}} \equiv \boldsymbol{k}/k \tag{2}$$

where

$$c_k \equiv \cos\theta_k \equiv [(\omega+m)/2\omega]^{1/2} \qquad s_k \equiv \sin\theta_k \equiv [(\omega-m)/2\omega]^{1/2}$$
$$\omega \equiv \omega_k \equiv (k^2+m^2)^{1/2}. \tag{3}$$

The plane-wave expansion of the electron–positron operator field is

$$\Psi_x = \int (2\pi)^{-3/2}\,\mathrm{d}\boldsymbol{k}\,\Psi_k\,\mathrm{e}^{-\mathrm{i}kx}$$

and Ψ_k can be expanded over the four eigenvectors of the Dirac Hamiltonian (1), that is over the four columns of the matrix $R(\boldsymbol{k})$ (2). The components corresponding to the positive eigenvalue are denoted b and are interpreted as bare electron destruction operators, while the components corresponding to the negative eigenvalue are denoted d^{+} and are interpreted as bare positron creation operators:

$$(\Psi_k) = R(\boldsymbol{k})\begin{pmatrix} b_k \\ d^{+}_{\bar{k}} \end{pmatrix} \qquad \bar{\boldsymbol{k}} \equiv -\boldsymbol{k}. \tag{4}$$

The operator b^{+}_k creates a charge $-e$ and a momentum $\boldsymbol{k}$, and the operator d^{+}_k creates a charge $+e$ and a momentum $\boldsymbol{k}$. Therefore b_k, $d^{\pm}_k$ and Ψ_k all correspond to an increment of momentum $-\boldsymbol{k}$, and to an increment of electric charge $+e$. The rotation $R(\boldsymbol{k})$ (4) between the Fourier component Ψ_k of the electron field and the bare particle operators b and d^{+} is a particular Bogoliubov transformation (see I), characterised by the 'bare vacuum Bogoliubov angle' θ_k (3). θ_k depends only on ω_k, and takes on values ranging from 0 to $\pi/4$. $\theta = 0$ corresponds to the static limit (the 'large' component c_k is large and the 'small' component s_k is small), and $\theta = \pi/4$ corresponds to the ultra-relativistic limit (the 'large' and 'small' components are of the same order of magnitude).

The bare vacuum is the Fock state $|0\rangle$ characterised by $b|0\rangle = d|0\rangle = 0$, and the Dirac sea is described by the projection operator upon the negative eigenvalue eigenstates of $h_{\mathrm{D}}(\boldsymbol{k})$, that is the vacuum expectation value of the tensor product $\Psi^{+}\otimes\Psi$:

$$\Lambda^{(-)} \equiv \langle 0|\Psi^{+}\otimes\Psi|0\rangle \equiv R\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}R^{+}. \tag{5}$$

A charge-conserving momentum-diagonal Bogoliubov transformation mixes the b's and d^+'s, and leads to dressed electron destruction operators $\tilde{b}$ and dressed positron creation operators $\tilde{d}^+$:

$$\begin{pmatrix} \tilde{b}_k \\ \tilde{d}^+_{\bar{k}} \end{pmatrix} = T(\boldsymbol{k}) \begin{pmatrix} b_k \\ d^+_{\bar{k}} \end{pmatrix} = \begin{pmatrix} \cos \eta_k & \sin \eta_k \\ -\sin \eta_k & \cos \eta_k \end{pmatrix} \begin{pmatrix} b_k \\ d^+_{\bar{k}} \end{pmatrix}. \tag{6}$$

This transformation combines with $R(\boldsymbol{k})$, leading to an expansion of the Fourier component Ψ_k of the electron field over a new basis:

$$(\Psi_k) = \tilde{R}(\boldsymbol{k}) \begin{pmatrix} \tilde{b}_k \\ \tilde{d}^+_{\bar{k}} \end{pmatrix} \tag{7}$$

where the matrix $\tilde{R} \equiv RT^+$ of the rotated wavefunctions is also momentum-diagonal:

$$\tilde{R}(\boldsymbol{k}) = \begin{pmatrix} \tilde{c}_k & -\tilde{s}_k(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{k}}) \\ \tilde{s}_k(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{k}}) & \tilde{c}_k \end{pmatrix} \tag{8}$$

with

$$\tilde{c}_k \equiv \cos(\eta_k + \theta_k) \qquad \tilde{s}_k \equiv \sin(\eta_k + \theta_k).$$

The vacuum $|\tilde{0}\rangle$ of the dressed particle operators is characterised by $\tilde{b}|\tilde{0}\rangle = \tilde{d}|\tilde{0}\rangle = 0$. It corresponds to the transformed Dirac sea described by its 'density matrix', which is the transformed projection operator $\tilde{\Lambda}^{(-)}(\boldsymbol{k})$:

$$\tilde{\Lambda}^{(-)} \equiv \langle \tilde{0}|\Psi^+ \otimes \Psi|\tilde{0}\rangle \equiv \tilde{R} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tilde{R}^+. \tag{9}$$

The vacuum density $\tilde{\rho}$ has been defined in I (§ 3) as the expectation value in the dressed vacuum $|\tilde{0}\rangle$ of the normally ordered tensor product $\mathcal{N}[\Psi^+ \otimes \Psi]$, where $\mathcal{N}$ is the normal ordering corresponding to the bare vacuum $|0\rangle$. Therefore, $\tilde{\rho}$ is the difference $\tilde{\Lambda}^{(-)} - \Lambda^{(-)}$ between the operators that project upon the transformed and initial Dirac seas, respectively. Here, $\tilde{\rho}$ is momentum-diagonal and expressed as

$$\tilde{\rho}(\boldsymbol{k}) \equiv \langle \tilde{0}|\mathcal{N}[\Psi^+ \otimes \Psi]|\tilde{0}\rangle = \begin{pmatrix} \tilde{s}_k^2 - s_k^2 & -(\tilde{s}_k\tilde{c}_k - s_k c_k)(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{k}}) \\ -(\tilde{s}_k\tilde{c}_k - s_k c_k)(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{k}}) & \tilde{c}_k^2 - c_k^2 \end{pmatrix}. \tag{10}$$

This density represents the modification of the Dirac sea under the action of the BDF transformation.

The Fock-space Hamiltonian under consideration has a term describing the kinetic energy, and a term describing the two-body interaction between the charges at different points $\boldsymbol{x}$ and $\boldsymbol{y}$:

$$H = \mathcal{N}\left[\int \mathrm{d}\boldsymbol{x}\, \Psi^+_x h_D \Psi_x + \int \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y}\, \mathcal{V}(\boldsymbol{x}-\boldsymbol{y})(\Psi^+_x \cdot \Psi_x)(\Psi^+_y \cdot \Psi_y) \right]. \tag{11}$$

Note that QED in Coulomb gauge leads to such an electron-positron Hamiltonian. Photons appear in other terms that do not contribute in the considered variational space.

In momentum space the Dirac operator is

$$h_D \begin{pmatrix} \boldsymbol{kq} \\ \alpha\beta \end{pmatrix} = h_D(\boldsymbol{k})_{\alpha\beta} \delta(\boldsymbol{k}-\boldsymbol{q}) \tag{12}$$

and the antisymmetrical scalar local two-body interaction can be written as

$$\mathcal{V} \begin{pmatrix} \boldsymbol{kqpr} \\ \alpha\beta\gamma\delta \end{pmatrix} = \tfrac{1}{2}[\mathcal{V}(\boldsymbol{p}-\boldsymbol{k})\delta_{\alpha\gamma}\delta_{\beta\delta} - \mathcal{V}(\boldsymbol{r}-\boldsymbol{k})\delta_{\alpha\delta}\delta_{\beta\gamma}]\delta(\boldsymbol{k}+\boldsymbol{q}-\boldsymbol{p}-\boldsymbol{r}) \tag{13}$$

where $\boldsymbol{k}$, $\boldsymbol{p}$, $\boldsymbol{q}$, $\boldsymbol{r}$ are momenta and α, β, γ, δ are bispinor component indices. The two terms in the square brackets are the direct and exchange contributions, respectively.

The energy $\tilde{E}_0 = \langle\tilde{0}|H|\tilde{0}\rangle$ of the dressed vacuum is infinite since a '$\delta(0)$' factor arises from integration over momentum. This infinite factor is interpreted as the volume of position space. As usual for translation-invariant problems, one works with the vacuum energy per unit of volume, which is $\tilde{\mathscr{E}}_0 \equiv \int \mathrm{d}\boldsymbol{k}\, \tilde{E}_0(\boldsymbol{k})$, with

$$\tilde{E}_0(\boldsymbol{k}) \equiv 4\left[m - \int \mathrm{d}\boldsymbol{q}\, \mathscr{V}(\boldsymbol{k}-\boldsymbol{q})(\tilde{s}_q^2 - s_q^2) \right](\tilde{s}_k^2 - s_k^2)$$
$$-4\left[k + \int \mathrm{d}\boldsymbol{q}\, \mathscr{V}(\boldsymbol{k}-\boldsymbol{q})(\tilde{s}_q\tilde{c}_q - s_q c_q)(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{q}}) \right](\tilde{s}_k\tilde{c}_k - s_k c_k). \tag{14}$$

As described in I, and as usual in mean-field theories, the stationarity equations involve a density $\tilde{\rho}$ and a mean-field Hamiltonian $\tilde{h}$. The BDF mean-field Hamiltonian is $\tilde{h} = h_D + \tilde{\Gamma}$, where $\tilde{\Gamma}$ is the vacuum polarisation potential due to the vacuum density. Here $\tilde{\Gamma}$ is expressed (summation over repeated indices is assumed) as

$$\tilde{\Gamma}\begin{pmatrix} \boldsymbol{kq} \\ \alpha\beta \end{pmatrix} = 4\mathscr{V}\begin{pmatrix} \boldsymbol{rkpq} \\ \delta\alpha\gamma\beta \end{pmatrix}\tilde{\rho}\begin{pmatrix} \boldsymbol{pr} \\ \gamma\delta \end{pmatrix}. \tag{15}$$

The direct part vanishes since the local charge is zero everywhere due to the translational invariance of the variational vacuum, and there only remains the exchange part

$$\tilde{\Gamma}\begin{pmatrix} \boldsymbol{kq} \\ \alpha\beta \end{pmatrix} = -2\delta(\boldsymbol{k}-\boldsymbol{q})\mathscr{V}(\boldsymbol{k}-\boldsymbol{p})\tilde{\rho}(\boldsymbol{p})_{\alpha\beta}. \tag{16}$$

This vacuum polarisation potential is momentum-diagonal, and therefore so will be the BDF Hamiltonian $\tilde{h} = h_D + \tilde{\Gamma}$, which can be written

$$\tilde{h}(\boldsymbol{k}) = \begin{pmatrix} M_k & \Delta_k \\ \Delta_k & -M_k \end{pmatrix} \tag{17}$$

where

$$M_k \equiv m - 2\int \mathrm{d}\boldsymbol{q}\, \mathscr{V}(\boldsymbol{k}-\boldsymbol{q})(\tilde{s}_q^2 - s_q^2)$$
$$\Delta_k \equiv (\boldsymbol{\sigma}\cdot\boldsymbol{k}) + 2\int \mathrm{d}\boldsymbol{q}\, \mathscr{V}(\boldsymbol{k}-\boldsymbol{q})(\tilde{s}_q\tilde{c}_q - s_q c_q)(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{q}}). \tag{18}$$

3. Gap equations

The stationarity condition for the BDF energy is the BDF equation

$$[\tilde{h}, \tilde{\Lambda}^{(-)}] = 0. \tag{19}$$

This implies that the rotation $\tilde{R}(\boldsymbol{k})$ (8) can be chosen to diagonalise simultaneously $\tilde{\Lambda}^{(-)}$ (9) and the BDF Hamiltonian $\tilde{h}(\boldsymbol{k})$. The matrix $\tilde{h}(\boldsymbol{k})$ transformed by $\tilde{R}(\boldsymbol{k})$ is

$$\tilde{R}^{+}\tilde{h}\tilde{R}$$
$$= \begin{pmatrix} \cos[2(\theta+\eta)]M + \sin[2(\theta+\eta)]\delta & \cos[2(\theta+\eta)]\Delta - \sin[2(\theta+\eta)]M(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}}) \\ \cos[2(\theta+\eta)]\Delta - \sin[2(\theta+\eta)]M(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}}) & -\cos[2(\theta+\eta)]M - \sin[2(\theta+\eta)]\delta \end{pmatrix}$$

where we have introduced

$$\delta_k \equiv \tfrac{1}{2}[\Delta_k(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}})+(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}})\Delta_k] = k + 2\int \mathrm{d}\boldsymbol{q}\, \mathcal{V}(\boldsymbol{k}-\boldsymbol{q})\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{q}}(\tilde{s}_q\tilde{c}_q - s_q c_q). \tag{20}$$

For each momentum $\boldsymbol{k}$, $\tilde{R}^+\tilde{h}\tilde{R}$ is diagonal when the off-diagonal terms vanish,

$$\cos[2(\theta+\eta)]\Delta - \sin[2(\theta+\eta)]M(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}}) = 0$$

which implies after multiplication on both sides by $\boldsymbol{\sigma}\cdot\hat{\boldsymbol{k}}$ that

$$\cos[2(\theta+\eta)]\delta - \sin[2(\theta+\eta)]M = 0.$$

The eigenvalues $\pm\lambda$ of the BDF Hamiltonian and the corresponding stationary Bogoliubov angles η (6) are characterised by (we repeat between parentheses definitions from (3) for comparison):

$$\begin{aligned} &\lambda_k^2 = M_k^2 + \delta_k^2 && (\omega_k^2 = m^2 + k^2) \\ &\sin[2(\theta_k+\eta_k)] = \delta_k/\lambda_k && (\sin(2\theta_k) = k/\omega_k) \\ &\cos[2(\theta_k+\eta_k)] = M_k/\lambda_k && (\cos(2\theta_k) = m/\omega_k). \end{aligned} \tag{21}$$

Since M and δ given by (18) and (20) are functionals of the angles η, equations (21) are functional equations for the BDF angle η. One can also get rid of the Bogoliubov angles by inserting the last two relations (21) into (18). One obtains a set of two integral equations for the functions M and δ, which determine the spectrum of the BDF Hamiltonian via the first relation of (21):

$$\begin{aligned} M_k &\equiv m - \int \mathrm{d}\boldsymbol{q}\, \mathcal{V}(\boldsymbol{k}-\boldsymbol{q})\left(\frac{m}{\omega_q} - \frac{M_q}{\lambda_q}\right) \\ \delta_k &\equiv k - \int \mathrm{d}\boldsymbol{q}\, \mathcal{V}(\boldsymbol{k}-\boldsymbol{q})\left(\frac{q}{\omega_q} - \frac{\delta_q}{\lambda_q}\right)\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{q}}. \end{aligned} \tag{22}$$

The equations (22) may be considered as a relativistic generalisation of the non-relativistic 'gap equations', characterising the changes in a mean-field spectrum due to pairing correlations (Bardeen *et al* 1957, Ring and Schuck 1980). The Hamiltonian (11), which is normally ordered with respect to the bare vacuum, can be reordered with respect to the variational dressed vacuum (I, § 4). Then, H is written as the sum of (i) the c-number $\tilde{E}_0$, (ii) a one-body term where the Dirac Hamiltonian h_D has been replaced by the BDF Hamiltonian $\tilde{h}$, and (iii) the residual two-body interaction. At the stationary point, that is when the gap equations are satisfied, this reduces to

$$H = \tilde{E}_0 + \int \mathrm{d}\boldsymbol{k}\, \lambda_k(\tilde{b}_k^+\tilde{b}_k + \tilde{d}_k^+\tilde{d}_k) + \text{residual two-body interaction.}$$

Therefore, the spectrum of the one-body part of the Hamiltonian *in the BDF representation* is given by the eigenvalues $\pm\lambda_k$ of the BDF Hamiltonian, and the relation $\lambda_k = (M_k^2+\delta_k^2)^{1/2}$ is the new dispersion relation between energy and momentum.

The gap equations (22) have the trivial solution $M_k = m$ and $\delta_k = k$. This means that the bare vacuum is a stationary point of the energy functional in the present variational space. However, this stationary point may be unstable and there may exist non-trivial solutions, depending on the form and intensity of the two-body interaction $\mathcal{V}$. In order to illustrate this, we may specify the two-body interaction (Coulomb interaction with a coupling constant α) and consider special forms of the functions

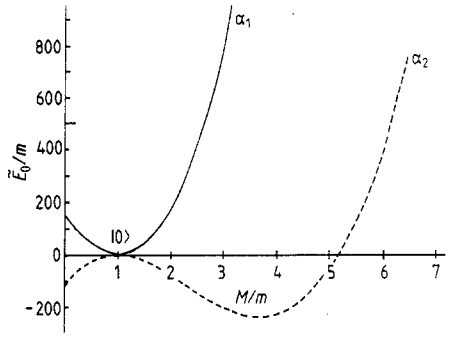

Figure 1. Vacuum energy in a restricted variational space of BDF states labelled by a single parameter M, for a Coulomb two-body interaction. Two values $\alpha_1 < \alpha_2$ of the coupling constant are considered. The bare vacuum corresponds to $M/m = 1$, and is a stationary point of the energy. For a small coupling constant α_1 the bare vacuum is stable against variations of M (full curve). For a large coupling constant α_2 the bare vacuum becomes unstable (broken curve); in this case, the energy exhibits a minimum for a given value of the parameter M. This minimum may itself be unstable within the complete BDF variational space (see § 4).

M_k and δ_k with two free parameters M and Λ (see § 4). We plot in figure 1 the BDF vacuum energy against M for a given value Λ and for two values α_1 and α_2 of the coupling constant α, such that $\alpha_1 < \alpha_2$. The bare vacuum corresponds to $M/m = 1$ and is always a stationary point. It is stable for $\alpha = \alpha_1$, at least within the considered restricted variational space (full curve). It becomes unstable for α_2 large enough (broken curve). In this latter case the BDF energy exhibits a new minimum, which is stable within the considered restricted variational space, but may be unstable in the complete BDF variational space (this is indeed what happens, as shown in § 4). As we shall see in the following two sections, this example shows that, provided the coupling constant is large enough, the vacuum is unstable in the BDF variational space, and *a fortiori* in the complete Fock space.

4. Minimisation of the BDF energy: the Coulomb case

We now restrict the discussion to a pure Coulomb interaction, and we look for a minimum of the BDF energy density $\tilde{E}_0$ (14). The two-body interaction $\mathcal{V}$ can be written as

$$\mathcal{V}(\boldsymbol{x}-\boldsymbol{y}) = \tfrac{1}{2}\alpha|\boldsymbol{x}-\boldsymbol{y}|^{-1}$$

or in momentum space

$$\mathcal{V}(\boldsymbol{k}-\boldsymbol{q}) = \tfrac{1}{2}\alpha(2\pi)^{-3}4\pi|\boldsymbol{k}-\boldsymbol{q}|^{-2} \tag{23}$$

where α is the electromagnetic coupling constant. In the following discussion, the coupling constant α as well as the electron-positron mass m are considered as parameters. The vacuum energy $\tilde{E}_0$ (14) is then a functional $\tilde{E}$ of the Bogoliubov angles η_k (6), and a function of the parameters α and m:

$$\tilde{E}_0 = \tilde{E}(m, \alpha, \eta). \tag{24}$$

We look for an infimum of $\tilde{E}(\alpha, m, \eta)$ as a functional of η:

$$I(m, \alpha) \equiv \inf_{\eta} \tilde{E}(m, \alpha, \eta). \tag{25}$$

The vacuum energy (24) can be written as

$$\tilde{E}(m, \alpha, \eta) = T(m, \eta) - \alpha(2\pi)^{-2} V(m, \eta) \tag{26}$$

where T corresponds to the kinetic part of the Hamiltonian and V to the two-body interaction. The kinetic energy is

$$T(m, \eta) = 4 \int \mathrm{d}\boldsymbol{k}\, \omega_k \sin^2 \eta_k \tag{27}$$

where ω_k is the kinetic energy of a particle with momentum $\boldsymbol{k}$, and $4 \sin^2 \eta_k$ is the number of particles with momentum $\boldsymbol{k}$ (there are two spin orientations for each particle, two particles in each pair and $\sin^2 \eta_k$ pairs for a given momentum $\boldsymbol{k}$ and a given spin orientation). Finally the potential energy is

$$V(m, \eta) = 4 \int \frac{\mathrm{d}\boldsymbol{k}\, \mathrm{d}\boldsymbol{q}}{|\boldsymbol{k} - \boldsymbol{q}|^2} \sin \eta_k \sin \eta_q [\sin(\eta_k + 2\theta_k) \sin(\eta_q + 2\theta_q) + \cos(\eta_k + 2\theta_k) \cos(\eta_q + 2\theta_q)\, \hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{q}}]. \tag{28}$$

Although the functional form $\mathcal{V}$ (23) of the two-body interaction does not depend on m, this parameter does appear in the Coulomb contribution $V(m, \eta)$ to the energy. This is due to the normal ordering, that is to the vacuum subtraction, which depends on m since the bare vacuum is defined relative to the free Dirac Hamiltonian.

The mass of the electron is the only scale parameter in the problem. This implies the following scaling behaviour:

$$\tilde{E}(m, \alpha, \eta(\cdot)) = \lambda^4 \tilde{E}(m/\lambda, \alpha, \eta(\lambda \cdot)). \tag{29}$$

Since $\eta(\cdot)$ and $\eta(\lambda \cdot)$ run over the same variational space, the infimum (25) fulfils

$$I(m, \alpha) = \lambda^4 I(m/\lambda, \alpha). \tag{30}$$

This scaling law has important consequences:

(i) For $\lambda = m$, this gives the scaling law $I(m, \alpha) = m^4 I(1, \alpha)$.

(ii) For $m = 0$, this gives $I(0, \alpha) = \lambda^4 I(0, \alpha)$ for every λ, and then, since $I(m, \alpha) \leqslant 0$, $I(0, \alpha)$ is either 0 or $-\infty$.

(iii) If $I(0, \alpha) = -\infty$, then $I(m, \alpha) = \lambda^4 I(m/\lambda, \alpha) = \lim_{\lambda \to \infty} \lambda^4 I(m/\lambda, \alpha) = -\infty$.

Since $V(m, \eta) \geqslant 0$, $I(m, \alpha)$ is a decreasing function of α. As a consequence, there exists a critical value $\alpha_c(m)$ such that $I(m, \alpha) = 0$ if $\alpha < \alpha_c(m)$, and $I(m, \alpha) < 0$ if $\alpha > \alpha_c(m)$. Because of (i), the critical value does not depend on m; therefore $\alpha_c(m) = \alpha_c(0) \equiv \alpha_c$. Because of (ii) and (iii),

$$I(m, \alpha) = 0 \qquad \text{if } \alpha < \alpha_c \tag{31}$$

$$I(m, \alpha) = -\infty \qquad \text{if } \alpha > \alpha_c. \tag{32}$$

Furthermore, one can see that $I(m, \alpha_c) = 0$; indeed, if $I(m, \alpha_c) = -\infty$ there exists a function η such that

$$T(m, \eta) - \alpha_c (2\pi)^{-2} V(m, \eta) = \tilde{E}(m, \alpha_c, \eta) \leqslant -\varepsilon < 0,$$

i.e

$$\alpha_c \geqslant (2\pi)^2 [\varepsilon + T(m, \eta)] / V(m, \eta).$$

Then let us consider

$$\alpha \equiv (2\pi)^2[\varepsilon/2 + T(m, \eta)]/V(m, \eta).$$

One has $\alpha < \alpha_c$, and

$$\tilde{E}(m, \alpha, \eta) = T(m, \eta) - \alpha(2\pi)^{-2}V(m, \eta) = -\varepsilon/2 \leqslant 0$$

which contradicts (31).

To summarise, we have shown that the BDF vacuum exhibits a stability-instability transition behaviour. There is a critical value $\alpha_c \geqslant 0$ of the coupling constant, independent of m, such that

$$\text{if } \alpha > \alpha_c \qquad \text{then } I(m, \alpha) = -\infty \tag{33}$$

$$\text{if } \alpha \leqslant \alpha_c \qquad \text{then } I(m, \alpha) = 0. \tag{34}$$

It is remarkable that α_c does not depend on the electron-positron mass m. This stems from the absence of scale in the two-body interaction.

We can conclude that the bare vacuum $|0\rangle$ is the lowest energy state of our variational space if the two-body Coulomb interaction is not too strong (that is if $\alpha < \alpha_c$). On the contrary, if α is large enough, the negative electron-positron Coulomb energy exceeds the sum of the kinetic energy and of the electron-electron and positron-positron repulsive energies. It then becomes energetically favourable to increase the Bogoliubov angles and the number of pairs in the vacuum. In this case the energy is not bounded below in the variational space.

In principle, like in perturbative field theory, the parameters α and m appearing in the Hamiltonian must be chosen to fit experimental values of observable quantities, for instance the physical electron mass m_e or a binding energy. This can lead to choosing input values of α and m that differ from $1/137$ and m_e, respectively, and these input values in general depend on the variational space. The problem of order-by-order renormalisation in perturbative theory is here replaced by the problem of non-perturbative renormalisation in a variational space. In the BDF variational space used for the description of the translationally invariant vacuum, the collapse for an overcritical input value of α occurs whatever the input value of m. Therefore no mass renormalisation will be able to compensate for it, that is to say that the input value of α has to be undercritical for the theory to make sense.

5. Bounds on the critical coupling constant

To ensure that the Hamiltonian (11) is bounded below in the electron-positron Fock space and that an atomic-structure calculation via a minimisation procedure is legitimate, it is necessary that the coupling constant α appearing in the Hamiltonian be undercritical. It is therefore necessary to look for bounds on α_c. A heuristic argument shows that one can expect α_c to be of the order of magnitude unity: the ground-state energy of a 'positron-electron' system, as given by the fine-structure formula with a reduced mass $m/2$, goes to zero when α goes to unity. Therefore, it becomes gradually easier to create a real pair when α approaches unity, and pairs will be spontaneously created for $\alpha > 1$. Greiner and coworkers (Reinhard *et al* 1971, Greiner *et al* 1985) have used and refined the argument, applied to the 'electron-external field' system: there the coupling constant is $Z\alpha$ ($\alpha = 1/137$, Z = nuclear charge), and the argument shows that spontaneous pair creation might occur for Z greater than a critical value

of the order $1/\alpha$. In our case, this kind of argument based on one-particle theory is unreliable. Since there is no simple general procedure to separate the motion of two interacting relativistic particles into a centre-of-mass motion and a relative motion with reduced mass (Bodwin *et al* 1985), the use of the fine-structure formula for positronium and with a large coupling constant is not justified. However we will give bounds on α_c, and show that indeed α_c is of the order of magnitude unity. First we give a finite upper bound on the critical coupling constant and therefore show that variational collapse in the BDF space may occur, provided that α is large enough. Next, we give a non-vanishing lower bound to the critical coupling constant, and show that the energy is stable in the BDF variational space provided that α is small enough.

5.1. Upper bound on α_c and possibility of variational collapse

Here we study the energy functional in a restricted variational space, and we consider Bogoliubov angles such that

for $k<\Lambda$ $\quad \cos\tilde{\theta}_k \equiv [(\Omega+M)/2\Omega]^{1/2} \qquad \sin\tilde{\theta}_k \equiv [(\Omega-M)/2\Omega]^{1/2}$

$\Omega_k \equiv (k^2+M^2)^{1/2}$

for $k \geqslant \Lambda$ $\quad \tilde{\theta}_k \equiv \theta_k$

where Λ and M are variational parameters.

In the restricted space, the energy functional $\tilde{E}(m, \alpha, \eta)$ (26) becomes a function $\tilde{E}(m, \alpha, \Lambda, M)$. One can check after tedious but straightforward calculations that, for a given M, the behaviour of $\tilde{E}$ for large Λ is

$$\tilde{E}(m, \alpha, \Lambda, M) = \frac{\pi}{4}\left(1-\frac{\ln 4}{\pi}\alpha\right)(M-m)^2\Lambda^2 + o(\Lambda^2). \tag{35}$$

This shows that if $\alpha > \pi/\ln 4$, $\tilde{E}$ has no minimum unbounded in the restricted space, and *a fortiori* in the complete Bogoliubov space. Therefore the critical coupling constant is finite, and $\alpha_c < \pi/\ln 4$.

As an illustration we can compute $\tilde{E}(m, \alpha, \Lambda, M)$ explicitly, and figure 1 represents $\tilde{E}$ as a function of M for a given value Λ_0 of the variational parameter Λ, and for two values α_1 and α_2 of the coupling constant α. (i) For $\alpha_1 < \pi/\ln 4$, one can see that $\tilde{E}(m, \alpha_1, \Lambda_0, M)$ is minimum for $M=m$, and the bare vacuum is stable; (ii) for $\alpha_2 > \pi/\ln 4$, the bare vacuum is unstable, and $\tilde{E}(m, \alpha_1, \Lambda_0, M)$ has a minimum for a non-trivial value $M_{\min}$ of the variational parameter M. However, the above analysis shows that the energy functional actually is not bounded below, and that the dressed vacuum corresponding to Λ_0 and $M_{\min}$ is unstable.

5.2. Lower bound on α_c and possibility of variational stability

The energy functional (26) can be bounded below in the following way:

$$\tilde{E}(m, \alpha, \eta) \geqslant T(m, \eta) - \alpha(2\pi)^{-2}|V(m, \eta)|. \tag{36}$$

Now, the kinetic energy increases with m:

$$T(m, \eta) = 4\int \mathrm{d}\boldsymbol{k}\, \omega_k \sin^2\eta_k \geqslant 4\int \mathrm{d}\boldsymbol{k}\, k \sin^2\eta_k \tag{37}$$

and on the other hand

$$|V(m,\eta)| \leqslant 4\int \frac{\mathrm{d}\boldsymbol{k}\,\mathrm{d}\boldsymbol{q}}{|\boldsymbol{k}-\boldsymbol{q}|^2}|\sin\eta_k||\sin\eta_q||\sin(\eta_k+2\theta_k)sin(\eta_q+2\theta_q) + \cos(\eta_k+2\theta_k)\cos(\eta_q+2\theta_q)\,\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{q}}|$$

where the last absolute value is smaller than unity since it is the scalar product of two normalised 4-vectors:

$$|V(m,\eta)| \leqslant 4\int \frac{\mathrm{d}\boldsymbol{k}\,\mathrm{d}\boldsymbol{q}}{|\boldsymbol{k}-\boldsymbol{q}|^2}|\sin\eta_k||\sin\eta_q|. \tag{38}$$

This majorisation is related to the fermionic character of the electron field, for which the densities are smaller than unity, and for which the squared density can be majorised by the density itself. Let $s(\boldsymbol{x})$ be the Fourier transform of $|\sin\eta_k|$; we have

$$\tilde{E}(m,\alpha,\eta) \geqslant 4\int \mathrm{d}\boldsymbol{x}\, s(\boldsymbol{x})[(-\Delta)^{1/2}-\tfrac{1}{2}\alpha|\boldsymbol{x}|^{-1}]s(\boldsymbol{x}). \tag{39}$$

Then we use the following lemma, which allows a comparison between kinetic and potential energies (a derivation of this lemma is outlined in a mathematical note in the appendix at the end of the paper).

Lemma. For any real function s such that $s(\boldsymbol{x})(-\Delta)^{1/2}s(\boldsymbol{x})$ is integrable over $\mathbb{R}^3$, then $s(\boldsymbol{x})|\boldsymbol{x}|^{-1}s(\boldsymbol{x})$ is also integrable over $\mathbb{R}^3$, and one has

$$\int \mathrm{d}\boldsymbol{x}\, s(\boldsymbol{x})|\boldsymbol{x}|^{-1}s(\boldsymbol{x}) \leqslant (\pi/2)\int \mathrm{d}\boldsymbol{x}\, s(\boldsymbol{x})(-\Delta)^{1/2}s(\boldsymbol{x}) \tag{40}$$

(furthermore $\pi/2$ is the smallest constant for which this inequality holds for every s).

Therefore, if $\alpha \leqslant 4/\pi$, then $\tilde{E}(m,\alpha,\eta) \geqslant 0$, and hence $I(m,\alpha)=0$. Then one can conclude that the critical coupling constant is greater than $4/\pi$.

Finally we showed that the critical coupling constant α_c satisfies:

$$4/\pi \leqslant \alpha_c < \pi/\ln 4. \tag{41}$$

The behaviour of the BDF vacuum energy depending on the numerical value of the coupling constant is summed up in figure 2. (From a somewhat different point of view, Hardekopf and Sucher (1985) analysed the question of spontaneous positronium creation on the basis of the no-pair two-particle theory, and found a critical coupling constant $\simeq 1.8$.)

It is noteworthy that (39) brought us back to the study of $(-\Delta)^{1/2}-\gamma|\boldsymbol{x}|^{-1}$, for a given value of the parameter γ. The '0 or $-\infty$' behaviour of the BDF vacuum energy is reminiscent of the 'stability-instability' alternative for this 'semi-relativistic' one-particle Hamiltonian $(-\Delta)^{1/2}-\gamma|\boldsymbol{x}|^{-1}$ (Kato 1966, Weder 1975, Herbst 1977a, b, Daubechies 1984). This Hamiltonian has been introduced in the mathematical physics literature as an ersatz of the one-particle Dirac-Coulomb Hamiltonian $\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m-\gamma|\boldsymbol{x}|^{-1}$, for $m=0$. It is remarkable that it occurs here, not as an ersatz, but in the study of a minimisation procedure applied to the Hamiltonian of QED. Therefore we have

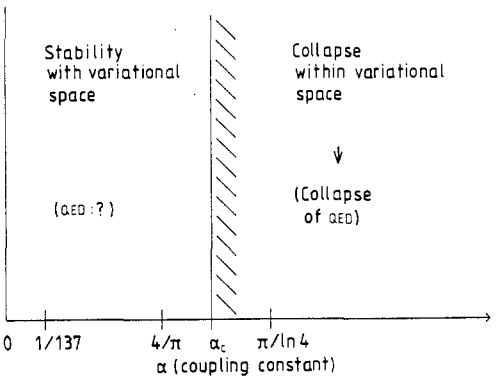

Figure 2. The stability of the BDF vacuum with a Coulomb two-body interaction depends on the value α assigned to the coupling constant. For α larger than the critical coupling constant α_c, the bare vacuum is unstable and the energy functional has no minimum. *A fortiori*, the Hamiltonian of QED in Coulomb gauge is not bounded below in this case. For α smaller than the critical value α_c, the bare vacuum is the translationally invariant uncharged Fock state of lowest energy, and the Hamiltonian is bounded below within the considered variational space. However, this does not mean that it is bounded below in the complete Fock space. It is shown in § 4 that the physical value $\alpha \simeq 1/137$ is undercritical.

here an unexpected interpretation of the results concerning the academic Hamiltonian $(-\Delta)^{1/2} - \gamma|\boldsymbol{x}|^{-1}$.

6. Concluding remarks

Since the physical value $\alpha \simeq 1/137$ is subcritical, the variational procedure leads one to choose the bare vacuum $|0\rangle$ for the description of the empty space in BDF theory. However, the collapse of the BDF vacuum energy for $\alpha > \alpha_c$ is of a more general significance. The BDF variational space is a subspace of the 'electron-positron' Fock space, and of the 'electron-positron-transverse photon' Fock space of Coulomb-gauge QED. If the BDF vacuum energy collapses in the BDF variational space, and this does happen for $\alpha > \alpha_c$, then *a fortiori* the complete Coulomb-gauge QED Hamiltonian is not bounded below. Since no photons are included in the BDF variational space, α_c cannot be considered as a reliable estimate of a possible critical value for the stability of Coulomb-gauge QED, but only as an upper bound: the critical value of the coupling constant for the collapse of QED is smaller than α_c.

This result may be compared to those deduced from perturbative approaches. The question of the stability of the bare vacuum in quantum-field theories where fermions are coupled via scalar or vector bosons has yet been addressed by several authors (Cohen *et al* 1987, Soni 1987). It can be shown within the perturbative approximation at the one-loop level that the bare vacuum is not the uncharged Fock state of lowest energy, even after one-loop renormalisation. Whether or not this instability of the bare vacuum is an artefact of the one-loop approximation remains an open question since higher-order terms of the perturbative expansions may change this result. Although it leaves the status of a 'renormalisation' in Hamiltonian non-perturbative quantum-field theory to be investigated, our demonstration of the collapse of Coulomb-gauge QED for a large enough coupling constant does not rely on a perturbative expansion; it

therefore gives a complementary view on the question of vacuum stability in quantum-field theory.

Appendix. Mathematical note

Here we outline a proof of the following result that we used in the study of the BDF vacuum.

Lemma. There exists a constant C such that for any smooth real function s with a compact support, we have

$$\int \mathrm{d}\boldsymbol{x}\, s(\boldsymbol{x})|\boldsymbol{x}|^{-1}s(\boldsymbol{x}) \leqslant C \int \mathrm{d}\boldsymbol{x}\, s(\boldsymbol{x})(-\Delta)^{1/2}s(\boldsymbol{x}).$$

By density, such an inequality holds for the homogeneous Sobolev space $\dot{\mathscr{H}}^{1/2,2}(\mathbb{R}^3)$, which is the closure of the space of compactly supported smooth real functions with respect to the norm

$$\|s\| = \left(\int \mathrm{d}\boldsymbol{x}\, s(\boldsymbol{x})(-\Delta)^{1/2}s(\boldsymbol{x}) \right)^{1/2}.$$

Furthermore, $C = \pi/2$ is the smallest constant such that the inequality holds for all s.

One proof of the above inequality relies on delicate convolution properties, and we only sketch it.

First of all, if s belongs to $\dot{\mathscr{H}}^{1/2,2}(\mathbb{R}^3)$, by Sobolev embeddings s belongs not only to $L^3(\mathbb{R}^3)$ but also to the Lorentz space $L^{3,2}(\mathbb{R}^3)$. Hence, s^2 belongs to $L^{3/2,1}(\mathbb{R}^3)$. Since $|\boldsymbol{x}|^{-1}$ belongs to $L^{3,\infty}(\mathbb{R}^3)$, by Hölder inequalities, the product $s^2(\boldsymbol{x})|\boldsymbol{x}|^{-1}$ belongs to $L^{1,1}(\mathbb{R}^3) = L^1(\mathbb{R}^3)$, that is $s(\boldsymbol{x})|\boldsymbol{x}|^{-1}s(\boldsymbol{x})$ is integrable over $\mathbb{R}^3$.

Since Sobolev embeddings define a continuous embedding from $\dot{\mathscr{H}}^{1/2,2}(\mathbb{R}^3)$ into $L^{3,2}(\mathbb{R}^3)$, the above argument also yields the existence of a positive constant C *independent of* s such that the above inequality holds.

For the value $C = \pi/2$, the inequality holds for every s: if it were not the case, one could find a positive real number E and a compactly supported smooth real function s, such that

$$\int \mathrm{d}\boldsymbol{x}\, s(\boldsymbol{x})[(-\Delta)^{1/2} - (2/\pi)|\boldsymbol{x}|^{-1}]s(\boldsymbol{x}) \leqslant -2E \qquad \int \mathrm{d}\boldsymbol{x}\, s^2(\boldsymbol{x}) = 1.$$

Introducing a decreasing sequence V_n of smooth compactly supported negative potentials such that

$$-(2/\pi)|\boldsymbol{x}|^{-1} \leqslant V_n \leqslant 0 \qquad V_n \to -(2/\pi)|\boldsymbol{x}|^{-1}$$

we could deduce by continuity that for n large enough

$$\int \mathrm{d}\boldsymbol{x}\, s(\boldsymbol{x})[(-\Delta)^{1/2} + V_n]s(\boldsymbol{x}) \leqslant -E \qquad \int \mathrm{d}\boldsymbol{x}\, s^2(\boldsymbol{x}) = 1.$$

Next, consider the ground state of $(-\Delta)^{1/2} + V_n$, which exists in view of the properties of V_n and the above inequality. It satisfies

$$[(-\Delta)^{1/2} + V_n]s_n = \varepsilon_n s_n \qquad \varepsilon_n \leqslant -E \qquad \int \mathrm{d}\boldsymbol{x}\, s_n^2(\boldsymbol{x}) = 1$$

and has a fixed sign, say positive (this characterisation of the fundamental is easy to prove for the Schrödinger operator $-\Delta+V$; in the present case, it follows from the fact that $\|t\| \leqslant \|s\|$ if $t \equiv |s|$, where the norm $\|\cdot\|$ has been defined above).

Multiplying this equation by $\underline{s}(x) \equiv |x|^{-1}$, which satisfies

$$[(-\Delta)^{1/2} - (2/\pi)|x|^{-1}]\underline{s}(x) = 0$$

and integrating by parts (integration which can be justified by a tedious argument), we deduce

$$\int \mathrm{d}x\, s_n(x)[(2/\pi)|x|^{-1} + V_n]|x|^{-1} = \varepsilon_n \int \mathrm{d}x\, |x|^{-1} s_n(x)$$

This is a contradiction since the first term is positive and the second one is negative.

In summary, we proved that

$$\int \mathrm{d}x\, s(x)|x|^{-1}s(x) \leqslant (\pi/2) \int \mathrm{d}x\, s(x)(-\Delta)^{1/2}s(x).$$

In this derivation, we used the fact that, in a loose sense, $\underline{s}(x)$ is the 'fundamental' of $(-\Delta)^{1/2} - (2/\pi)|x|^{-1}$, with zero eigenvalue. This implies that $C = \pi/2$ actually is the smallest C value for which this inequality holds.

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