A variational model for relativistic electrons

Mathieu LEWIN

Mathieu.Lewin@math.cnrs.fr

(CNRS & Université de Cergy-Pontoise)

joint works with C. Hainzl (Birmingham, Alabama), P. Gravejat, É. Séré (Paris Dauphine, France) & J.-P. Solovej (Copenhagen, Denmark)

Seminari di fisica matematica, Università di Pisa, June 10th, 2008

References

[HLS1] C. Hainzl, M. L. & E. Séré. Existence of a stable polarized vacuum in the Bogoliubov-Dirac-Fock approximation, *Commun. Math. Phys.* (2005).

[HLS2] C. Hainzl, M. L. & E. Séré. Self-consistent solution for the polarized vacuum in a no-photon QED model. *J. Phys. A: Math & Gen.* (2005).

[HLSo] C. Hainzl, M. L. & J.P. Solovej. The mean-field approximation in Quantum Electrodynamics. The no-photon case. *Comm. Pure Appl. Math.* (2007).

[HLS3] C. Hainzl, M. L. & E. Séré. Existence of Atoms and Molecules in the Mean-Field Approximation of No-Photon QED, *Arch. Rat. Mech. Anal.* (2008).

[GLS] P. Gravejat, M. L. & E. Séré. Ground State and Charge Renormalization in a Nonlinear Model of Relativistic Atoms, `arXiv:0712.2911`.

[Rev] C. Hainzl, M. L., E. Séré and J.P. Solovej. A Minimization Method for Relativistic Electrons in a Mean-Field Approximation of Quantum Electrodynamics, *Phys. Rev. A* (2007).

The free Dirac operator

- Energy of a free electron ($p \longleftrightarrow -i\nabla$)

	non relativistic	relativistic
classical mechanics	$E = p^2/(2m)$	$E^2 = c^2p^2 + m^2c^4$
quantum mechanics	$H = -\Delta/(2m)$	$D^2 = -c^2\Delta + m^2c^4$

- Free Dirac operator ('28):

$$\boxed{D^0 = -ic\sum_{k=1}^{3}\alpha_k\partial_k + \beta mc^2 = -ic\boldsymbol{\alpha}\cdot\nabla + \beta mc^2}$$

$\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are 4×4 self-adjoint matrices satisfying the CAR

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij}, \qquad \alpha_i\beta + \beta\alpha_i = 0.$$

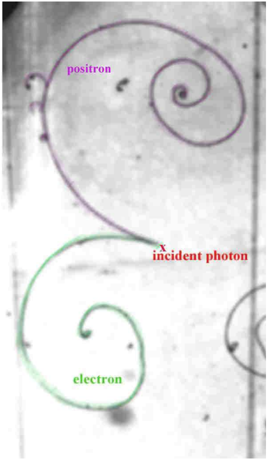
D^0 is defined on $L^2(\mathbb{R}^3, \mathbb{C}^4)$ with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and

$$(D^0)^2 = -c^2\Delta + m^2c^4.$$

It is *unbounded from below*:

$$\sigma(D^0) = (-\infty; -mc^2] \cup [mc^2; +\infty).$$

Dirac's interpretation of the negative spectrum



Spontaneaous creation of an electron-positron pair.
Source: `www.cern.ch`

Dirac (1934): *"We make the assumption that, in the world as we know it, nearly all the states of negative energy for the electrons are occupied, with just one electron in each state, and that a uniform filling of all the negative-energy states is completely unobservable to us."*

$\rightarrow$ **Vacuum = Dirac sea** = infinitely many virtual electrons occupying the negative energies.

- can feel an external field and will react accordingly $\rightarrow$ **Vacuum Polarization.**
- if the external field is strong enough, **electron-positron pairs** can be created.

Here: a model describing the *coupled system* "real electrons + Dirac sea".

Summary

- A nonlinear functional $Q \mapsto \mathcal{E}(Q)$ whose variable Q is a self-adjoint operator of infinite rank ($\rightarrow$ *infinitely many particles to describe*).
- A locally compact problem, but with possible loss of compactness at infinity;

  $\rightarrow$ *need to adapt usual arguments from nonlinear analysis. Constraint on operator Q hard to deal with, in particular regarding localization issues.*
- We will look for minimizers, possibly under a constraint;

  $\rightarrow$ *would be interesting to study other critical points & time-dependent equation [HLSp] ($\rightarrow$ description of spontaneous creation of electron-positron pairs).*
- model contains many divergences which have a physical interpretation

  $\rightarrow$ *linked to renormalization in QED.*

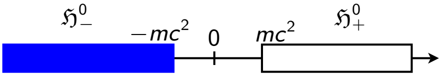
[HLSp] C. Hainzl, M. L. & C. Sparber. Existence of global-in-time solutions to a generalized Dirac-Fock type evolution equation, *Lett. Math. Phys.* (2005).

Hartree-Fock states

- **State of the system** = an orthogonal projector P acting on $L^2(\mathbb{R}^3, \mathbb{C}^4)$.
  - $\text{Rank}(P)$ = number of particles (electrons);
  - if $(\varphi_i)_{i\in I}$ is an orthonormal basis of $\text{Ran}(P)$, $P = \sum_{i\in I} |\varphi_i\rangle\langle\varphi_i|$, then φ_i's = states of the individual electrons.

Exemples. Introduce $P_-^0 = \chi_{(-\infty;0)}(D^0)$ and $P_+^0 = 1 - P_-^0$. Let $(\varphi_i^\pm)_i$ be an orthonormal basis of $\mathfrak{H}_\pm^0 := P_\pm^0 L^2(\mathbb{R}^3, \mathbb{C}^4)$.

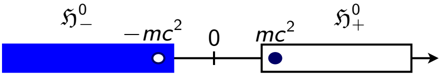
Free Dirac sea



$$P = P_-^0 = \sum_{i=1}^{\infty} |\varphi_i^-\rangle\langle\varphi_i^-|$$

$$Q = P - P_-^0 = 0$$

An electron-positron pair



$$P = P_-^0 - |\varphi_1^-\rangle\langle\varphi_1^-| + |\varphi_1^+\rangle\langle\varphi_1^+|$$

$$Q = -|\varphi_1^-\rangle\langle\varphi_1^-| + |\varphi_1^+\rangle\langle\varphi_1^+|.$$

- **Units in the following:** $\hbar = m = c = 1$, $\alpha = e^2$ (fine structure cst).

Hartree-Fock (formal) energy

Formal Energy in the state P:

$$\mathcal{E}^\nu(P - P^0_-) = \operatorname{tr}(D^0(P - P^0_-)) - \alpha \iint \frac{\rho_{P-P^0_-}(x)\nu(y)}{|x-y|}dx\,dy + \frac{\alpha}{2}\iint \frac{\rho_{P-P^0_-}(x)\rho_{P-P^0_-}(y)}{|x-y|}dx\,dy$$

Here: $\rho_\Gamma(x) = \operatorname{tr}_{\mathbb{C}^4}(\Gamma(x,x))$.

- May be derived from no-photon QED by means of a thermodynamic limit [HLSo]. Was introduced by Chaix-Iracane (*J. Phys. B* '89) and mathematically studied by Bach-Barbaroux-Helffer-Siedentop (*CMP* '99) for $\nu = 0$. Then Hainzl-L.-Séré for $\nu \neq 0$.
- This energy is (formally) convex. But we have neglected one term for the simplicity of this talk which is indeed not convex.
- We will see that if $\nu \equiv 0$, then $0 = P^0_- - P^0_-$ is the unique minimizer $\longrightarrow$ free Dirac vacuum.

A generalization of the trace

- **Pb:** there is no minimizer in the trace-class.
- **Ultraviolet cut-off** will be very useful

$$\mathfrak{H}_\Lambda = \{f \in L^2(\mathbb{R}^3;\mathbb{C}^4),\ \mathrm{supp}(\widehat{f}) \subset B(0;\Lambda)\}.$$

Definition. A Hilbert-Schmidt operator $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ is P^0_--trace class ($\in \mathfrak{S}_1^{P^0_-}(\mathfrak{H}_\Lambda)$) if $Q^{++} := P^0_+ Q P^0_+$ and $Q^{--} := P^0_- Q P^0_-$ are trace-class. We then define its P^0_--trace as $\mathrm{tr}_{P^0_-}(Q) := \mathrm{tr}(Q^{++} + Q^{--})$.

Theorem (Properties of P^0_--trace [HLS1])

(i) Let $Q = P - P^0_-$ with $P = P^* = P^2$. Then $P - P^0_- \in \mathfrak{S}_1^{P^0_-}(\mathfrak{H}_\Lambda) \Leftrightarrow P - P^0_- \in \mathfrak{S}_2$ and in this case $\mathrm{tr}_{P^0_-}(P - P^0_-)$ is an integer.

(ii) Let P be an orthogonal projector acting on $\mathfrak{H}_\Lambda$ such that $P - P^0_- \in \mathfrak{S}_2$. Then $\mathfrak{S}_1^{P^0_-}(\mathfrak{H}_\Lambda) = \mathfrak{S}_1^{P}(\mathfrak{H}_\Lambda)$ and $\mathrm{tr}_{P^0_-}(Q) = \mathrm{tr}_P(Q)$ for every Q.

Idea. When $P - P^0_- \in \mathfrak{S}_1^{P^0_-}(\mathfrak{H}_\Lambda)$, then $\mathrm{tr}_{P^0_-}(P - P^0_-)$ =charge of the state.

Density

• **Density.** $\rho_Q(x) = \mathrm{tr}_{\mathbb{C}^4}(Q(x,x))$ is well-defined $\forall Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ since $\mathrm{Supp}\ \widehat{Q} \subseteq B(0,\Lambda)^2 \Rightarrow Q(x,y)$ smooth.
We introduce:

$$D(f,g) := 4\pi \int_{\mathbb{R}^3} |k|^{-2}\overline{\widehat{f}(k)}\widehat{g}(k), \qquad \mathcal{C} := \{f \mid D(f,f) < \infty\}.$$

Lemma (Definition of the density [HLS3])

$\Lambda > 0$. The map $Q \in \mathfrak{S}_1^{P^0_-}(\mathfrak{H}_\Lambda) \mapsto \rho_Q \in L^2 \cap \mathcal{C}$ is continuous, i.e. there exists a constant $C = C(\Lambda)$ such that:

$$\|\rho_Q\|_{L^2} + D(\rho_Q,\rho_Q)^{1/2} \leq C\left(\|Q\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)} + \|Q^{++}\|_{\mathfrak{S}_1(\mathfrak{H}_\Lambda)} + \|Q^{--}\|_{\mathfrak{S}_1(\mathfrak{H}_\Lambda)}\right).$$

Rmk. If Q is trace-class, then $\rho_Q \in L^1(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} \rho_Q = \mathrm{tr}_{P^0_-}(Q) = \mathrm{tr}(Q).$$

We will see that this does *not* hold for a minimizer of $\mathcal{E}^\nu$.

Definition of the BDF Energy

$$\boxed{\mathcal{E}^\nu(Q) := \mathrm{tr}_{P^0_-}(D^0 Q) - \alpha D(\nu, \rho_Q) + \frac{\alpha}{2} D(\rho_Q, \rho_Q)}$$

$$Q \in \mathcal{Q}_\Lambda := \left\{ Q \in \mathfrak{S}_1^{P^0_-}(\mathfrak{H}_\Lambda) \mid Q^* = Q, \ -P^0_- \leq Q \leq P^0_+ \right\}.$$

(Convex hull of $\{Q = P - P^0_- \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\}$, cf Lieb, PRL '81)

Lemma (The BDF Energy is bounded-below)

$\alpha \geq 0$, $\Lambda > 0$, $\nu \in \mathcal{C}$. *The functional $\mathcal{E}^\nu$ is well-defined on $\mathcal{Q}_\Lambda$. It satisfies*

$$\forall Q \in \mathcal{Q}_\Lambda, \qquad \mathcal{E}^\nu(Q) + \frac{\alpha}{2} D(\nu, \nu) \geq 0$$

and it is thus bounded-below. If moreover $\nu = 0$, then $\mathcal{E}^0$ is nonnegative, 0 being its unique minimizer.

Proof: Notice $-P^0_- \leq Q \leq P^0_+ \iff Q^2 \leq Q^{++} - Q^{--}$ and
$\mathrm{tr}_{P^0_-}(D^0 Q) = \mathrm{tr}(|D^0|(Q^{++} - Q^{--})) \geq \mathrm{tr}(Q^{++} - Q^{--}) \geq \mathrm{tr}(Q^2) \geq 0.$

Existence of the Polarized Vacuum

Theorem (Definition of the Polarized Vacuum [HLS2])

Let $\alpha \geq 0$, $\Lambda > 0$, $\nu \in \mathcal{C}$. *The functional* $\mathcal{E}^\nu$ *possesses a global minimizer* $\bar{Q}$ *on* $\mathcal{Q}_\Lambda$. *It is not necessarily unique but its density* $\rho_{\bar{Q}}$ *is uniquely defined; it is radially symmetric if* ν *is radially symmetric.*
The operator $\bar{Q}$ *is a solution of the self-consistent equation*

$$\begin{cases} \bar{Q} = \chi_{(-\infty,0)}\left(D_{\bar{Q}}\right) - P^0_- + \delta \\ D_{\bar{Q}} = D^0 + \alpha\left(\rho_{\bar{Q}} - \nu\right) * \dfrac{1}{|\cdot|} \end{cases} \tag{1}$$

where $0 \leq \delta \leq 1$ *is finite rank and satisfies* $\mathrm{Ran}(\delta) \subseteq \ker(D_Q)$.
Moreover, if α *and* ν *satisfy* $\alpha\pi^{1/6}2^{11/6}D(\nu,\nu)^{1/2} < 1$, *then* $\ker(D_Q) = \{0\}$, *hence* $\delta = 0$ *and* $\bar{Q}$ *is unique. In this case the associated vacuum is neutral:* $\mathrm{tr}_{P^0_-}(\bar{Q}) = 0$.

Proof of the existence: $\mathcal{E}^\nu$ is wlsc for the weak-$*$ topology of $\mathfrak{S}_1^{P^0_-}(\mathfrak{H}_\Lambda)$.

Renormalization

When $\nu \neq 0$, a self-consistent solution $\bar{Q}$ of (1) is *not trace-class*.

Theorem (L^1 regularity and renormalization [GLS])

Let $\alpha \geq 0$, $\Lambda > 0$, $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3)$ with $Z = \int_{\mathbb{R}^3} \nu$. Let $\bar{Q}$ be a self-consistent solution of (1). Then $\rho_{\bar{Q}} \in L^1(\mathbb{R}^3)$ and

$$\boxed{\int_{\mathbb{R}^3} \rho_{\bar{Q}} - Z = \frac{\mathrm{tr}_{P^0_-}(\bar{Q}) - Z}{1 + \alpha B_\Lambda}} \qquad (2)$$

where $B_\Lambda = \frac{2}{3\pi} \log \Lambda - \frac{5}{9\pi} + \frac{2 \log 2}{3\pi} + O(1/\Lambda^2)$.

Renormalization. Assume for instance $\alpha \pi^{1/6} 2^{11/6} D(\nu,\nu)^{1/2} < 1$. Then $\mathrm{tr}_{P^0_-}(\bar{Q}) = 0$ but $\int \rho_{\bar{Q}} \neq 0$. Observed density: $\nu - \rho_{\bar{Q}}$. Potential observed far away: $e_{\rm phys} Z/|x|$ where

$$\boxed{e_{\rm phys} = \frac{e}{1 + \alpha B_\Lambda}} \qquad \text{(well-known in QED).}$$

Close to the nucleus, different behavior like the oscillations of $\rho_{\bar{Q}}$.

The First Order Density

- Assume $\alpha\pi^{1/6}2^{11/6}D(\nu,\nu)^{1/2} < 1$ and **drop the nonlinear term**:
$Q = \chi_{(-\infty,0]}(D^0 - \alpha\nu * |\cdot|^{-1}) - P^0_-$ (Furry picture). Then

$$Q = -\frac{\alpha}{2\pi}\int_{-\infty}^{\infty}\frac{1}{D^0+i\eta}(-\nu*|\cdot|^{-1})\frac{1}{D^0+i\eta}d\eta + \alpha^2 Q_2$$

with $Q_2 \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)$ and $\mathrm{tr}(Q_2) = \mathrm{tr}_{P^0_-}(Q) = 0$. Then, in Fourier space

$$\widehat{\rho_Q}(k) = -\alpha B_\Lambda(k)(-\widehat{\nu})(k) + \alpha^2\widehat{\rho_2}(k)$$

with the logarithmically divergent function (notation $E(p) = \sqrt{1+|p|^2}$)

$$B_\Lambda(k) = -\frac{1}{\pi^2|k|^2}\int_{\substack{|\ell+k/2|\leq\Lambda,\\ |\ell-k/2|\leq\Lambda}}\frac{(\ell+k/2)\cdot(\ell-k/2)+1-E(\ell+k/2)E(\ell-k/2)}{E(\ell+k/2)E(\ell-k/2)(E(\ell+k/2)+E(\ell-k/2))}d\ell.$$

- For a **nonlinear solution**, $-\nu \leftrightarrow \rho_{\bar{Q}} - \nu$, hence

$$\widehat{\rho_Q}(k) - \widehat{\nu}(k) = \frac{-1}{1+\alpha B_\Lambda(k)}\widehat{\nu}(k) + \alpha^2\frac{\widehat{\rho_2}(k)}{1+\alpha B_\Lambda(k)}$$

Rmk. Renormalization well interpreted within the nonlinear model. Does not work if the nonlinear term is neglected. Open with the exchange term.

Minimization in Charge Sectors

Let $\mathcal{Q}_\Lambda(q) := \{Q \in \mathcal{Q}_\Lambda,\ \mathrm{tr}_{P^0_-}(Q) = q\}$. Define

$$\boxed{E^\nu(q) := \inf \{\mathcal{E}^\nu(Q) \mid Q \in \mathcal{Q}_\Lambda(q)\}}$$

Theorem (Existence of atoms and molecules [HLS3,GLS])

Assume $\alpha \geq 0$, $\Lambda > 0$, $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3)$ with $Z = \int_{\mathbb{R}^3} \nu \in \mathbb{R}$. Then there exists $q_m < q_M$ such that

(i) $[q_m, q_M]$ is the largest interval on which $q \to E^\nu(q)$ is strictly convex;

(ii) the interval $[q_m, q_M]$ contains both Z and the unique minimizer q_0 of $q \to E^\nu(q)$;

(iii) if $q \notin [q_m, q_M]$, then $\mathcal{E}^\nu$ has no minimizer in the charge sector $\mathcal{Q}_\Lambda(q)$;

(iv) if $q \in [q_m, q_M]$, then $\mathcal{E}^\nu$ has a minimizer Q in $\mathcal{Q}_\Lambda(q)$. It is not a priori unique but its density ρ_Q is uniquely determined. It is radial if ν is radial.

Minimization in Charge Sectors

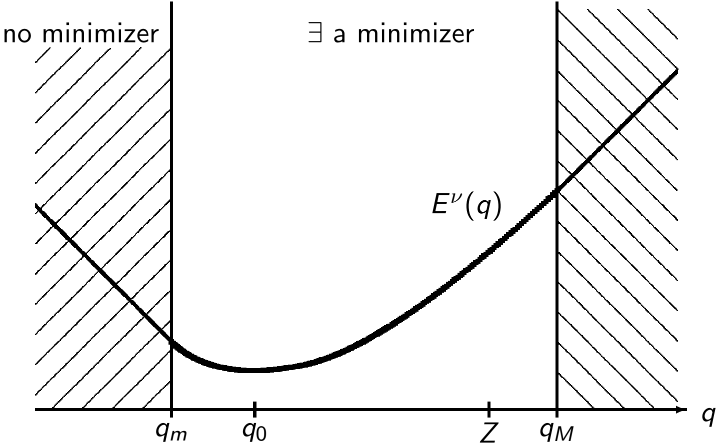
The operator Q satisfies the self-consistent equation

$$\begin{cases} Q + P^0_- = \chi_{(-\infty,\mu)}(D_Q) + \delta, \\ D_Q = D^0 + \alpha(\rho_Q - \nu) * |\cdot|^{-1}, \end{cases}$$

where $\mu \in [-1,1]$ is a Lagrange multiplier associated with the charge constraint and $0 \leq \delta \leq 1$ satisfies $\mathrm{Ran}(\delta) \subseteq \ker(D_Q - \mu)$.
Moreover, ρ_Q belongs to $L^1(\mathbb{R}^3)$ and satisfies (2).

Rmk. With the exchange term, this is more difficult [HLS3]. Proof of the existence if some binding conditions are fulfilled. We checked them in the non relativistic and the weak-coupling limit.

Minimization in Charge Sectors



Ionization estimate

Theorem (Ionization estimate [GLS])

For α small enough, $\nu \in L^1(\mathbb{R}^3) \cap \mathcal{C}$ with $\nu \geq 0$, $\int_{\mathbb{R}^3} \nu = Z$ and $\alpha D(\nu, \nu)$ small enough, we have

$$-C \frac{\alpha \log \Lambda + 1/\Lambda + \alpha D(\nu,\nu)}{1 - C\alpha \log \Lambda} \leq q_m \leq 0$$

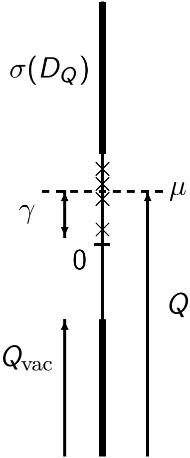
and

$$Z \leq q_M \leq \frac{2Z + C\left(\alpha \log \Lambda + 1/\Lambda + \alpha D(\nu,\nu)\right)}{1 - C\alpha \log \Lambda}.$$

Rmk. In the nonrelativistic limit $\alpha \to 0$ and $\Lambda \to \infty$ such that $\alpha \log \Lambda \to 0$, this reduces to an estimate of Lieb (PRA '84)

$$0 = q_m \leq Z \leq q_M \leq 2Z.$$

Interpretation of the Equation



Decomposition real particles / Dirac sea: Assume $q = N \in \mathbb{N}$ and $\alpha\pi^{1/6}2^{11/6}D(\nu,\nu)^{1/2} < 1$. Then ($\delta = 0$ for simplicity)

$$Q = \chi_{(-\infty;0]}(D_Q) - P^0_- + \chi_{(0;\mu]}(D_Q) = Q_{\rm vac} + \gamma,$$

$$\gamma = \sum_{i=1}^{N} |\varphi_i\rangle\langle\varphi_i|$$

with $\boxed{D_Q\varphi_i = \epsilon_i\varphi_i}$

and where $\epsilon_1 \leq \cdots \leq \epsilon_N$ are the N first positive eigenvalues of D_Q.

$$D_Q = D^0 + \alpha(\rho_\gamma - \nu) * |\cdot|^{-1} + \alpha\rho_{Q_{\rm vac}} * |\cdot|^{-1}$$

→ Dirac-Fock-type equations, perturbed by the Vacuum Polarization potential. Obtained through a minimization procedure, whereas the DF energy is strongly indefinite (cf Esteban-Séré).

References

[HLS1] C. Hainzl, M. L. & E. Séré. Existence of a stable polarized vacuum in the Bogoliubov-Dirac-Fock approximation, *Commun. Math. Phys.* (2005).

[HLS2] C. Hainzl, M. L. & E. Séré. Self-consistent solution for the polarized vacuum in a no-photon QED model. *J. Phys. A: Math & Gen.* (2005).

[HLSo] C. Hainzl, M. L. & J.P. Solovej. The mean-field approximation in Quantum Electrodynamics. The no-photon case. *Comm. Pure Appl. Math.* (2007).

[HLS3] C. Hainzl, M. L. & E. Séré. Existence of Atoms and Molecules in the Mean-Field Approximation of No-Photon QED, *Arch. Rat. Mech. Anal.* (2008).

[GLS] P. Gravejat, M. L. & E. Séré. Ground State and Charge Renormalization in a Nonlinear Model of Relativistic Atoms, arXiv:0712.2911.

[Rev] C. Hainzl, M. L., E. Séré and J.P. Solovej. A Minimization Method for Relativistic Electrons in a Mean-Field Approximation of Quantum Electrodynamics, *Phys. Rev. A* (2007).