Construction of the self-consistent Dirac vacuum in electromagnetic fields

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joint work with Philippe GRAVEJAT, Christian HAINZL and Mathieu LEWIN (arxiv.org/ 1204.2893)

The Dirac operator

The free Dirac operator ('28):

$$D_{m,0} = -i \sum_{k=1}^{3} \alpha_k \partial_k + \beta m = -i\boldsymbol{\alpha} \cdot \nabla + \beta m$$

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

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

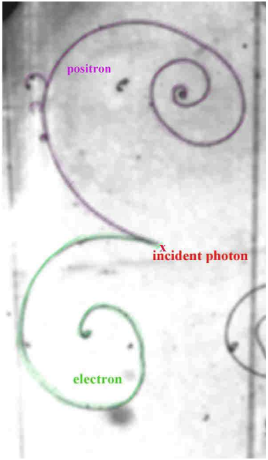
$D_{m,0}$ is defined on $L^2(\mathbb{R}^3, \mathbb{C}^4)$ with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and

$$(D_{m,0})^2 = -\Delta + m^2 .$$

It is *unbounded from below*:

$$\sigma(D_{m,0}) = (-\infty; -m] \cup [m; +\infty).$$

Dirac's interpretation of the negative continuous 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.

Consequence: real electrons can only occupy positive energy states.

The polarized Dirac sea

We consider a classical electromagnetic field $\mathbf{A} = (V, A)$. The associated Dirac operator is

$$D_{m,e\mathbf{A}} = \sum_{k=1}^{3} \alpha_k(-i\partial_k - eA_k) + \beta m - eV$$

Dirac sea = a one-body density matrix $0 \leq \Gamma \leq 1$ acting on $L^2(\mathbb{R}^3, \mathbb{C}^4)$. In its ground state, Γ is a projector of infinite rank:

$$\Gamma = \chi_{(-\infty,0)}(D_{m,e\mathbf{A}})$$

The mean-field (formal) action

Our variables are a one-body electronic density matrix $0 \leq \Gamma \leq 1$ and a classical electromagnetic field $\mathbf{A} = (V, A)$. The formal action of $(\Gamma, \mathbf{A})$ in the external field $\mathbf{A}_{\rm ext} = (V_{\rm ext}, A_{\rm ext})$ is:

$$\mathcal{S}^{\mathbf{A}_{\rm ext}}(\Gamma, \mathbf{A}) = \mathrm{tr}\left(D_{m,e(\mathbf{A}+\mathbf{A}_{\rm ext})}(\Gamma - 1/2)\right) + \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(|\mathrm{curl}\, A(x)|^2 - |\nabla V(x)|^2\right) dx. \tag{1}$$

Taking $\Gamma = \chi_{(-\infty,0]}(D_{m,e(\mathbf{A}+\mathbf{A}_{\rm ext})})$ one gets the (formal) *effective action*

$$\mathcal{L}^{\mathbf{A}_{\rm ext}}(\mathbf{A}) = -\frac{1}{2}\,\mathrm{tr}\left|D_{m,e(\mathbf{A}+\mathbf{A}_{\rm ext})}\right| + \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(|\mathrm{curl}\, A(x)|^2 - |\nabla V(x)|^2\right) dx. \tag{2}$$

Of course $\mathrm{tr}\left|D_{m,e(\mathbf{A}+\mathbf{A}_{\rm ext})}\right|$ is infinite. One can try to replace it by

$$\mathrm{tr}\left(\left|D_{m,e(\mathbf{A}+\mathbf{A}_{\rm ext})}\right| - \left|D_{m,0}\right|\right)$$

but the resulting trace is still ill-defined: an ultraviolet regularization is needed.

The Pauli-Villars ultraviolet regularization

A naive ultraviolet cut-off consists in replacing $L^2(\mathbb{R}^3;\mathbb{C}^4)$ by the space

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

This approach fails completely in presence of a magnetic field, because it breaks gauge invariance, and leads to divergences which behave quadratically in Λ. Instead we use the Pauli-Villars regularization:

$$\begin{aligned}\mathcal{L}_{PV}^{\mathbf{A}_{\rm ext}}(\mathbf{A}) = & -\frac{1}{2}\,\mathrm{tr}\,\Big\{\sum_{j=0}^{J} c_j\big(|D_{m_j,e(\mathbf{A}+\mathbf{A}_{\rm ext})}| - |D_{m_j,0}|\big)\Big\} \\ & + \frac{1}{8\pi}\int_{\mathbb{R}^3}\big(|\mathrm{curl}\,A(x)|^2 - |\nabla V(x)|^2\big)\,dx.\end{aligned} \tag{3}$$

Here $m_0 = m$ and $c_0 = 1$, whereas the other c_j and m_j describe fictitious particles with very large masses $m_j \gg 1$ such that

$$\sum_{j=0}^{J} c_j = \sum_{j=0}^{J} c_j\, m_j^2 = 0. \tag{4}$$

The Pauli-Villars auxiliary masses

For condition (4) to be fulfilled, at least two additional distinct masses m_1 and m_2 are necessary. When there are exactly two fictitious fields, the condition (4) is equivalent to

$$c_1 = \frac{m_0^2 - m_2^2}{m_2^2 - m_1^2} \quad \text{and} \quad c_2 = \frac{m_1^2 - m_0^2}{m_2^2 - m_1^2}. \tag{5}$$

We will always assume that $m_0 < m_1 < m_2$, which implies that $c_1 < 0$ and $c_2 > 0$.

In the limit $m_1, m_2 \to \infty$, the regularization does not prevent a logarithmic divergence, which is best understood in terms of the averaged ultraviolet cut-off Λ defined as

$$\log(\Lambda^2) := -\sum_{j=0}^{2} c_j \log(m_j^2). \tag{6}$$

The value of Λ does not determine m_1 and m_2 uniquely. In practice, the latter are chosen as functions of Λ such that c_1 and c_2 remain bounded when Λ goes to infinity.

Functional setting for the Pauli-Villars effective action

The question is to provide a rigorous meaning to the functional

$$\boxed{\mathcal{F}_{\rm PV}(\mathbf{A}) := \frac{1}{2}\,\mathrm{tr}\sum_{j=0}^{2} c_j\Big(\big|D_{m_j,0}\big| - \big|D_{m_j,\mathbf{A}}\big|\Big)} \tag{7}$$

for a general four-potential $\mathbf{A} = (V, A)$ in the Coulomb-gauge homogeneous Sobolev space

$$\dot{H}_{\rm div} := \Big\{\mathbf{A} = (V, A) \in L^6(\mathbb{R}^3, \mathbb{R}^4) \ : \\ \mathrm{div} A = 0 \text{ and } \mathbf{F} = (-\nabla V, \mathrm{curl}\, A) \in L^2(\mathbb{R}^3, \mathbb{R}^6)\Big\}, \tag{8}$$

endowed with its norm

$$\|\mathbf{A}\|^2_{\dot{H}_{\rm div}} := \|\nabla V\|^2_{L^2(\mathbb{R}^3)} + \|\mathrm{curl}\, A\|^2_{L^2(\mathbb{R}^3)} = \|\mathbf{F}\|^2_{L^2(\mathbb{R}^3)}. \tag{9}$$

Rigorous definition of the Pauli-Villars effective action

(i) Let $T_{\mathbf{A}} := \frac{1}{2}\sum_{j=0}^{2} c_j\Big(\big|D_{m_j,0}\big| - \big|D_{m_j,\mathbf{A}}\big|\Big)$. If $\mathbf{A} \in L^1(\mathbb{R}^3,\mathbb{R}^4)\cap \dot{H}_{\rm div}$, the operator $\mathrm{tr}_{\mathbb{C}^4}\, T_{\mathbf{A}}$ is trace-class on $L^2(\mathbb{R}^3,\mathbb{C})$. In particular, $\mathcal{F}_{\rm PV}(\mathbf{A})$ is well-defined in this case, by

$$\boxed{\mathcal{F}_{\rm PV}(\mathbf{A}) := \mathrm{tr}\,\big(\,\mathrm{tr}_{\mathbb{C}^4}\, T_{\mathbf{A}}\big).} \tag{10}$$

(ii) The functional $\mathcal{F}_{\rm PV}$ has a unique continuous extension to $\dot{H}_{\rm div}$ which takes the form

$$\boxed{\mathcal{F}_{\rm PV}(\mathbf{A}) = \mathcal{F}_2(-\nabla V, \mathrm{curl}\, A) + \mathcal{R}(\mathbf{A}),} \tag{11}$$

where $\mathcal{F}_2$ is a quadratic form, and the remainder $\mathcal{R}$ satisfies

$$|\mathcal{R}(\mathbf{A})| \leq K\left(\left(\sum_{j=0}^{2}\frac{|c_j|}{m_j}\right)\|\mathbf{A}\|^4_{\dot{H}_{\rm div}} + \left(\sum_{j=0}^{2}\frac{|c_j|}{m_j^2}\right)\|\mathbf{A}\|^6_{\dot{H}_{\rm div}}\right), \tag{12}$$

for a universal constant K.

Sign and logarithmic divergence of the second-order term

(iv) The functional $\mathcal{F}_2(E,B)$ is a bounded quadratic form on $L^2(\mathbb{R}^3,\mathbb{R}^4)$ given by

$$\mathcal{F}_2(E,B) = \frac{1}{8\pi}\int_{\mathbb{R}^3} M(k)\left(\left|\widehat{B}(k)\right|^2 - \left|\widehat{E}(k)\right|^2\right) dk, \tag{13}$$

where

$$M(k) := -\frac{2}{\pi}\sum_{j=0}^{2} c_j \int_0^1 u(1-u)\log\left(m_j^2 + u(1-u)|k|^2\right) du. \tag{14}$$

The function M is positive and satisfies the uniform estimate

$$0 < M(k) \leq M(0) = \frac{2\log(\Lambda)}{3\pi}, \tag{15}$$

where Λ was defined previously in (6).

Stability of the free vacuum

In the absence of an external field, the effective action is

$$\mathcal{L}^0_{PV}(\mathbf{A}) = \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(|B(x)|^2 - |E(x)|^2\right)dx + e^2\mathcal{F}_2(E,B) + \mathcal{R}(e\mathbf{A})$$

where $B = \operatorname{curl} A$ and $E = -\nabla V$.
The four-potential $\mathbf{A} \equiv 0$ is a saddle point of $\mathcal{L}^0_{PV}$. It is the unique solution of the min-max problem

$$\mathcal{L}^0_{PV}(0,0) = \max_{\|\nabla V\|_{L^2} < \frac{r\sqrt{m_0}}{e}} \mathcal{L}^0_{PV}(V,0) = \min_{\|\operatorname{curl} A\|_{L^2} < \frac{r\sqrt{m_0}}{e}} \mathcal{L}^0_{PV}(0,A), \quad (16)$$

or, equivalently,

$$\begin{aligned}\mathcal{L}^0_{PV}(0,0) &= \min_{\|\operatorname{curl} A\|_{L^2} < \frac{r\sqrt{m_0}}{e}} \ \sup_{\|\nabla V\|_{L^2} < \frac{r\sqrt{m_0}}{e}} \mathcal{L}^0_{PV}(V,A) \\ &= \max_{\|\nabla V\|_{L^2} < \frac{r\sqrt{m_0}}{e}} \ \inf_{\|\operatorname{curl} A\|_{L^2} < \frac{r\sqrt{m_0}}{e}} \mathcal{L}^0_{PV}(V,A),\end{aligned} \quad (17)$$

for some r which can be fixed if $\sum_{j=0}^2 |c_j|(m_0/m_j)$ and e remain bounded.

Polarized vacuum in small external fields

Now the effective action is

$$\mathcal{L}_{PV}^{\mathbf{A}_{\rm ext}}(\mathbf{A}) = \frac{1}{8\pi}\int_{\mathbb{R}^3}\left(|\mathrm{curl}\, A(x)|^2 - |\nabla V(x)|^2\right)dx + e^2\mathcal{F}_2(E+E_{\rm ext}, B+B_{\rm ext}) + \mathcal{R}(e\mathbf{A}+e\mathbf{A}_{\rm ext})\ . \tag{18}$$

(i) If $e\|\mathbf{A}_{\rm ext}\|_{\dot{H}_{\rm div}} < \frac{r\sqrt{m_0}}{8}$, there exists a unique solution $\mathbf{A}_* = (V_*, A_*)$ in $\dot{H}_{\rm div}$ of the min-max problem

$$\mathcal{L}_{PV}^{\mathbf{A}_{\rm ext}}(\mathbf{A}_*) = \max_{\|\nabla V\|_{L^2} < \frac{r\sqrt{m_0}}{4e}} \mathcal{L}_{PV}^{\mathbf{A}_{\rm ext}}(V, A_*) = \min_{\|\mathrm{curl}\, A\|_{L^2} < \frac{r\sqrt{m_0}}{4e}} \mathcal{L}_{PV}^{\mathbf{A}_{\rm ext}}(V_*, A)$$

The density and current of the Dirac sea

Given $\mathbf{A} \in \dot{H}_{\rm div}$, if 0 is not an eigenvalue of the operators $D_{m_j,\mathbf{A}}$, then the density $\rho_{\mathbf{A}}$ and current $j_{\mathbf{A}}$ of the polarized vacuum are defined as

$$\rho_{\mathbf{A}}(x) := \left[\operatorname{tr}_{\mathbb{C}^4} Q_{\mathbf{A}}\right](x,x) \quad \text{and} \quad j_{\mathbf{A}}(x) := \left[\operatorname{tr}_{\mathbb{C}^4}\ Q_{\mathbf{A}}\right](x,x), \tag{19}$$

and with $Q_{\mathbf{A}}$ referring to the kernel of the operator

$$Q_{\mathbf{A}} := \sum_{j=0}^{2} c_j \, \mathbb{1}_{(-\infty,0)}\big(D_{m_j,\mathbf{A}}\big).$$

The operators $\operatorname{tr}_{\mathbb{C}^4} Q_{\mathbf{A}}$ and $\operatorname{tr}_{\mathbb{C}^4} \alpha_k Q_{\mathbf{A}}$ for $k = 1, 2, 3$ are locally trace-class on $L^2(\mathbb{R}^3, \mathbb{C}^4)$, and $\rho_{\mathbf{A}}$ and $j_{\mathbf{A}}$ are well-defined functions in $L^1_{\rm loc}(\mathbb{R}^3) \cap \mathcal{C}$, where $\mathcal{C}$ is the Coulomb space

$$\mathcal{C} := \left\{ f : \mathbb{R}^3 \to \mathbb{C} : \int_{\mathbb{R}^3} \frac{|\widehat{f}(k)|^2}{|k|^2}\, dk < \infty \right\} = \dot{H}^{-1}(\mathbb{R}^3). \tag{20}$$

The self-consistent equations

(ii) The four-potential $\mathbf{A}_*$ is a solution of the nonlinear equations

$$\begin{cases} -\Delta V_* = 4\pi e \, \rho_{\mathbf{A}_* + \mathbf{A}_{\rm ext}}, \\ -\Delta A_* = 4\pi e \, j_{\mathbf{A}_* + \mathbf{A}_{\rm ext}}, \end{cases} \tag{21}$$

where $\rho_{\mathbf{A}_* + \mathbf{A}_{\rm ext}}$ and $j_{\mathbf{A}_* + \mathbf{A}_{\rm ext}}$ refer to the charge and current densities associated with the operator

$$Q_* = \sum_{j=0}^{2} c_j \, \mathbb{1}_{(-\infty,0)}\big(D_{m_j, e(\mathbf{A}_* + \mathbf{A}_{\rm ext})}\big). \tag{22}$$

Open questions

Can one extend this model to nonzero charge sectors?

Can one prove that the min-max principle is global?

Can one include the exchange term in this model?

Can one study a time-dependent version of this model?

It should be possible to study the charge renormalization, as in the case of no-photon mean-field QED.