Renormalization of Dirac's polarized vacuum

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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:

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

$\vec{\boldsymbol{\alpha}} = (\alpha_1, \alpha_2, \alpha_3)$, $\beta = 4\times 4$ hermitian matrices, chosen such that

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

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

Units: $m = c = 1$, $\alpha = e^2$.

A nonlinear Dirac equation

Stationary equation including Vacuum Polarization effects:

$$\begin{cases} P = \chi_{(-\infty,\mu)}(D) \\ D = D^0 + \alpha(\rho_{P-1/2} - \nu) * |x|^{-1} + X_P \end{cases} \qquad (1)$$

$$\begin{array}{r|l} \alpha = e^2 & \text{(bare) fine structure constant} \\ \nu & \text{charge density of nucleus (ex: } \nu = Z\delta_0) \\ \mu & \text{chemical potential chosen to fix total charge} \end{array}$$

$$X_P = \begin{cases} -\alpha\frac{(P-1/2)(x,y)}{|x-y|} & \textit{(Hartree-Fock Theory)} \\ 0 & \textit{(Reduced Hartree-Fock Theory)} \\ \frac{\partial F_{xc}}{\partial \rho}(\rho_{P-1/2}) & \textit{(Relativistic Density Functional Theory)} \end{cases}$$

- Density $\rho_Q(x) := \mathrm{tr}_{\mathbb{C}^4}(Q(x,x))$

[Dir34] P.A.M. Dirac. *Solvay report* XXV, 1934.
[EngDre87] Engel and Dreizler, *Phys. Rev. A*, 1987.

Interpretation

$$\begin{cases} P = \chi_{(-\infty,\mu)}(D) \\ D = D^0 + \alpha(\rho_{P-1/2} - \nu) * |x|^{-1} + 0 \end{cases} \quad (1)$$

- $\underline{\boldsymbol{\nu \equiv 0}}$ solution $P = P^0_- := \chi_{(-\infty,0)}(D^0)$ *(free vacuum)*, $\forall \mu \in (-1,1)$.

  Reason: $P^0_- - \frac{1}{2} = -\frac{\vec{\alpha}\cdot p + \beta}{2\sqrt{1+|p|^2}} \implies \rho_{P^0_- - 1/2} \equiv 0$.

  Rmk: For HF the free vacuum is different [HaiLewSol07].

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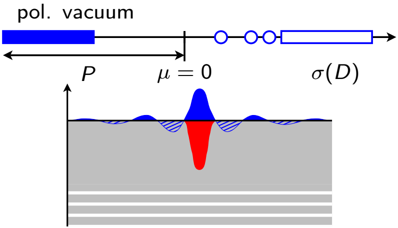
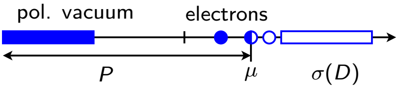
- $\underline{\boldsymbol{\nu \neq 0}}$

polarized vacuum



polarized vacuum + electrons



$\simeq$ Dirac-Fock eqs including Vacuum Polarization [ChaIra89]

[HaiLewSol07] Hainzl, L. and Solovej. *Comm. Pure Applied Math.* (2007).
[ChaIra89] Chaix and Iracane. *J. Phys. B* (1989).

Difficulties & Outline

- There is **no solution** to the nonlinear equation (1) when $\nu \neq 0$!
  - need to add an ultraviolet cut-off Λ
  - renormalization

- Possible to add classical SCF magnetic field ($\simeq$ photons), but no mathematical result so far.

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Outline

- Existence and non-existence of solutions
- Renormalization

Existence, nonperturbative regime

Regularization: Π_Λ= orth. projector onto $\mathfrak{H}_\Lambda = \{f \in L^2(\mathbb{R}^3;\mathbb{C}^4)\ :\ \text{supp}(\widehat{f}) \subset B(0;\Lambda)\}$. Define $\mathcal{C} := \{f\ :\ \int |\widehat{f}(k)|^2/|k|^2 < \infty\}$.

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Theorem (Existence [HaiLewSer05,GraLewSer09])

For all $\mu \in (-1,1)$, $\alpha \geq 0$, $\Lambda > 0$ and $\nu \in \mathcal{C}$, there exists **one solution** *to*

$$\begin{cases} P = \chi_{(-\infty,\mu)}(D) + \delta \\ D = \Pi_\Lambda \left(D^0 + \alpha(\rho_{P-P^0_-} - \nu) * \frac{1}{|x|} \right) \Pi_\Lambda \end{cases} \tag{2}$$

where $0 \leq \delta \leq \mathbb{1}_{\{\mu\}}(D)$, such that

$$P - P^0_- \in \mathfrak{S}_2, \qquad P^0_\pm(P - P^0_-)P^0_\pm \in \mathfrak{S}_1, \qquad \rho_{P-P^0_-} \in L^2 \cap \mathcal{C}.$$

- *All such solutions share the same density $\rho_{P-P^0_-}$.*
- *If $\alpha\pi^{1/6}2^{11/6}\,\|\nu\|_{\mathcal{C}} < 1$ and $\mu = 0$, then $\delta = 0$ and $P = P^2$ is unique. In this case $\mathrm{tr}\, P^0_-(P - P^0_-)P^0_- + P^0_+(P - P^0_-)P^0_+ = 0$.*

[HaiLewSer05] Hainzl, L. and Séré. *Comm. Math. Phys. + J. Phys. A: Math & Gen.* (2005).
[GraLewSer09] Gravejat, L. and Séré. *Comm. Math. Phys.* (2009).

Idea of proof ($\mu = 0$): variational method

- Subtract infinite constant, using $\rho_{P^0_- - 1/2} \equiv 0$ and $Q = P - P^0_-$

  "$\mathcal{E}^\nu_{\rm HF}(P - 1/2) - \mathcal{E}^\nu_{\rm HF}(P^0_- - 1/2)$" $=$

$$\mathrm{tr}\, D^0 Q - \alpha \iint \frac{\rho_Q(x)\nu(y)}{|x-y|} dx\, dy + \frac{\alpha}{2} \iint \frac{\rho_Q(x)\rho_Q(y)}{|x-y|} dx\, dy := \mathcal{E}^\nu_{\rm BDF}(Q)$$

- Then [BacBarHelSie99], notice $Q^2 = Q^{++} - Q^{--}$ and

$$\mathrm{tr}\, D^0 Q = \mathrm{tr}\, |D^0|(Q^{++} - Q^{--}) = \mathrm{tr}\, |D^0| Q^2$$

- Minimize the convex fn $\mathcal{E}^\nu_{\rm BDF}$ on the convex hull [Lie81]

$$\{Q = Q^* \ : \ Q^2 \leq Q^{++} - Q^{--} \in \mathfrak{S}_1\}$$

- The map $\{Q = Q^* \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \ : \ Q^{\pm\pm} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\} \mapsto \rho_Q \in L^2 \cap \mathcal{C}$ is continuous

- For $\mu \neq 0$, replace D^0 by $D^0 - \mu$

[BacBarHelSie99] Bach, Barbaroux, Helffer and Siedentop. *Comm. Math. Phys.* (1999).
[Lie81] Lieb. *Phys. Rev. Lett.* (1981).

Charge

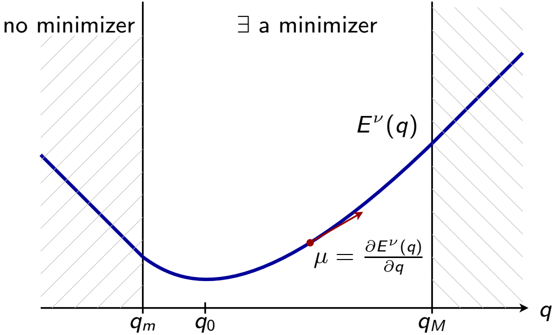
- We define the charge of our solution as

$$\mathrm{tr}_{P^0_-}(Q) := \mathrm{tr}\, P^0_- Q P^0_- + P^0_+ Q P^0_+$$

Rmk. if $P^2 = P$, then $\mathrm{tr}_{P^0_-}(P - P^0_-) \in \mathbb{Z}$, [AvrSeiSim94,HaiLewSer05]

- By convexity,

choosing μ ⇝ solving $E^\nu(q) := \inf\{\mathcal{E}^\nu_{\mathrm{BDF}}(Q),\ \mathrm{tr}_{P^0_-}(Q) = q\}$



[AvrSeiSim94] Avron, Seiler and Simon. *J. Funct. Anal.* (1994).

Maximum ionization

Theorem (Maximum Ionization [GraLewSer-09])

Assume $\nu \in \mathcal{C} \cap L^1$ *with* $Z := \int \nu$.

- *Then* $Z \in [q_m; q_M]$ *(existence of neutral atoms).*
- *For* $\alpha \|\nu\|_{\mathcal{C}} + \alpha(1 + \log \Lambda) \leq C'$ *and* $Z \geq 0$, *one has*

$$-C \frac{\alpha \log \Lambda + 1/\Lambda + \alpha \|\nu\|_{\mathcal{C}}}{1 - C\alpha \log \Lambda} \leq q_m \leq 0$$

and

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

Generalizes a result of Lieb in the nonrelativistic setting [Lie84].

[Lie84] Lieb. *Phys. Rev. A* (1984).

Renormalization

- **(Bare) parameters:** charge e ($\alpha = e^2$) and mass $m(= 1)$
  Regularization: UV cut-off Λ

  $\Rightarrow$ predicted observables = functions $\mathcal{O}(\alpha, \Lambda)$

- **Predicted charge / coupling constant:** $\alpha_{\rm ph}(\alpha, \Lambda) \neq \alpha$

- **Renormalization formulae:** see α as fn of $(\alpha_{\rm ph}, \Lambda)$

$$\alpha_{\rm ph} = \alpha_{\rm ph}(\alpha, \Lambda) \Longrightarrow \alpha = \alpha(\alpha_{\rm ph}, \Lambda)$$

  $\Rightarrow$ predicted observables = functions $\mathcal{O}(\alpha_{\rm ph}, \Lambda)$

- **Renormalization:** 'remove' Λ from observable $\mathcal{O}(\alpha_{\rm ph}, \Lambda)$
(possibly only perturbatively in $\alpha_{\rm ph}$)

Charge renormalization

Theorem (Charge renormalization [GraLewSer-09])

Assume that $\nu \in L^1(\mathbb{R}^3) \cap \mathcal{C}$ *with* $Z = \int \nu$, $\Lambda > 0$, $\alpha \geq 0$ *and* $\mu \in (-1, 1)$. *Then* $\rho_{P-P^0_-} \in L^1(\mathbb{R}^3)$ *and it holds*

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

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

- Except in neutral case, solutions are singular: $P - P^0_- \notin \mathfrak{S}_1$
- For $\|\nu\|_{\mathcal{C}}$ small, $\mu = 0$, observe $\alpha_{\rm ph} Z$ and not αZ, with

$$\alpha_{\rm ph} = \frac{\alpha}{1 + \alpha B_\Lambda} \iff \alpha = \frac{\alpha_{\rm ph}}{1 - \alpha_{\rm ph} B_\Lambda}$$

Pb (Landau pole): $\alpha_{\rm ph} B_\Lambda < 1$, hence $\Lambda \to \infty \Rightarrow \alpha_{\rm ph} \to 0$.

Self-consistent equation

- Assume $\mu = 0$ and $\ker(D) = \{0\}$. Cauchy's formula:

$$P - P^0_- = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\eta \left(\frac{1}{D + i\eta} - \frac{1}{D^0 + i\eta}\right)$$

We get in Fourier space

$$\widehat{\rho}_{P-P^0_-}(k) = -\alpha B_\Lambda(k)\big(\widehat{\rho}_{P-P^0_-}(k) - \widehat{\nu}(k)\big) + \widehat{F}_\Lambda\big(\alpha(\rho_{P-P^0_-} - \nu)\big) \qquad (4)$$

where

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

and $F_\Lambda(f) = \sum_{n\geq 1} F_{2n+1,\Lambda}(f,\dots,f)$ with

$$F_{k,\Lambda}(f_1,\dots,f_k) = \rho\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{D^0+i\eta}\prod_{j=1}^{k}\left(\Pi_\Lambda f_j * \frac{1}{|x|}\Pi_\Lambda\frac{1}{D^0+i\eta}\right)d\eta\right]$$

Renormalized equation

- **Renormalized density:** $\rho_{\rm ph} = \rho_{\rm ph}(\alpha_{\rm ph}, \Lambda)$ defined for $\alpha_{\rm ph} B_\Lambda < 1$ by

$$\alpha(\nu - \rho_{P-P^0_-}) = \alpha_{\rm ph}\rho_{\rm ph}$$

such that $D = D^0 - \alpha_{\rm ph}\rho_{\rm ph} * |\cdot|^{-1}$

- We can re-express Eq. (4) in terms of physical quantities as

$$(1 - \alpha_{\rm ph} U_\Lambda(k))\widehat{\rho}_{\rm ph} + \widehat{F}_\Lambda(\alpha_{\rm ph}\rho_{\rm ph}) = \widehat{\nu}$$

where $U_\Lambda(k) = B_\Lambda(0) - B_\Lambda(k) \geq 0$

Rmk.

$$\lim_{\Lambda\to\infty} U_\Lambda(k) = \frac{|k|^2}{4\pi}\int_0^1 \frac{z^2 - z^4/3}{1+|k|^2(1-z^2)/4}dz := U(k) \sim_{|k|\to\infty} \frac{2}{3\pi}\log|k|$$

[HaiLewSer05b] C. Hainzl, M.L. and É. Séré. *J. Phys. A: Math & Gen.*, 2005.
[Ueh35] E.A. Uehling. *Phys. Rev.*, 1935.

Renormalization in perturbation theory

- At least formally, we can write

$$\rho_{\rm ph}(\alpha_{\rm ph}, \Lambda) = \sum_{n\geq 0} (\alpha_{\rm ph})^n \nu_{n,\Lambda}$$

where $\begin{cases} \widehat{\nu}_{0,\Lambda} = \widehat{\nu}\mathbb{1}_{B(0,2\Lambda)}, \quad \widehat{\nu}_{1,\Lambda} = U_\Lambda(k)\widehat{\nu}_0(k), \\ \widehat{\nu}_{n,\Lambda} = U_\Lambda \widehat{\nu}_{n-1,\Lambda} + \sum_{j=3}^{n} \sum_{n_1+\cdots+n_j=n-j} \widehat{F}_{j,\Lambda}(\nu_{n_1,\Lambda}, ..., \nu_{n_j,\Lambda}) \text{ for } n\geq 2 \end{cases}$

- **Limit $\Lambda\to\infty$ in recursion formula** $\Rightarrow$ sequence $\{\nu_n\}_{n\geq 0}$

$$\nu_0 = \nu \quad \text{and} \quad \nu_1 * \frac{1}{|x|} = \frac{1}{3\pi}\int_1^\infty dt\,(t^2-1)^{1/2}\left[\frac{2}{t^2}+\frac{1}{t^4}\right]\int_{\mathbb{R}^3} e^{-2|x-y|t}\frac{\nu(y)}{|x-y|}\,dy$$

is the Uehling potential

Question: CV of series $\sum_{n\geq 0}(\alpha_{\rm ph})^n\nu_n$? probably divergent [Dys52]

[Dys52] F.J. Dyson. *Phys. Rev.*, 1952.

Asymptotic renormalization

Think of $\alpha_{\rm ph}$ and $\kappa := \alpha_{\rm ph} B_\Lambda$ as new parameters

Theorem (Asymptotics as $\alpha_{\rm ph} \to 0$ [GraLewSer10])

Let $\mu = 0$ and $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ such that, for some $N \geq 1$,

$$\int_{\mathbb{R}^3} \log(1 + |k|)^{2N+4} |\widehat{\nu}(k)|^2 \, dk < \infty.$$

Let $\epsilon > 0$. There exist two constants $C(\nu, N, \epsilon)$ and $a(\nu, N, \epsilon)$ depending on N, ν and ϵ such that one has

$$\left\| \rho_{\rm ph}(\alpha_{\rm ph}, \Lambda) - \sum_{n=0}^{N} (\alpha_{\rm ph})^n \nu_n \right\|_{L^2(\mathbb{R}^3) \cap \mathcal{C}} \leq C(\nu, N, \epsilon) \, (\alpha_{\rm ph})^{N+1}$$

for all $0 \leq \alpha_{\rm ph} \leq a(\nu, N, \epsilon)$ with $\epsilon \leq \alpha_{\rm ph} B_\Lambda \leq 1 - \epsilon$.

In terms of $\alpha_{\rm ph}$ and $\kappa \Rightarrow \Lambda \sim e^{3\kappa\pi/2\alpha_{\rm ph}}$ with $\epsilon \leq \kappa \leq 1 - \epsilon$.

[GraLewSér10] Gravejat, M.L. and Séré. `arXiv:1004.1734`

Conclusion

- Simple effective model for relativistic atoms including vacuum polarization
- Renormalization can be performed asymptotically
- Not a quantitative theory, but first step towards more advanced models

Open problems:

- Divergence of series $\sum_{n\geq 0}(\alpha_{\rm ph})^n\nu_n$?
- Include electromagnetic field
- Numerics