An alternative approach to the Dirac operator via the Dirichlet to Neumann operator

Margherita Nolasco

DISIM- Università dell' Aquila

Linear and Nonlinear Dirac Equation: advances and open problems

Como, February 8–10, 2017

[joint work with Vittorio Coti Zelati – Università di Napoli Federico II]

The Dirac operator

The (free) Dirac operator is a first order operator acting on 4-*spinors* $\Psi : \mathbb{R}^3 \to \mathbb{C}^4$, given by

$$D_0 = -ic\hbar \underline{\boldsymbol{\alpha}} \cdot \nabla + mc^2 \boldsymbol{\beta}$$

where c denotes the speed of light, $m > 0$ the mass of the electron, and $\hbar$ the Planck's constant (from now on $\hbar = 1$).

$\underline{\boldsymbol{\alpha}} = (\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3)$ and $\boldsymbol{\beta}$ are the four Pauli-Dirac 4×4-matrices, given by

$$\boldsymbol{\alpha}_k = \begin{pmatrix} 0 & \boldsymbol{\sigma}_k \\ \boldsymbol{\sigma}_k & 0 \end{pmatrix} \qquad \boldsymbol{\beta} = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}$$

and $\boldsymbol{\sigma}_k$ $(k = 1, 2, 3)$ are the Pauli 2×2-matrices.

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In Fourier space D_0 becomes the *multiplication* operator given by

$$\hat{D}(p) = \mathcal{F} D_0 \mathcal{F}^{-1} = \begin{pmatrix} mc^2 \mathbb{I}_2 & c\underline{\boldsymbol{\sigma}} \cdot p \\ c\underline{\boldsymbol{\sigma}} \cdot p & -mc^2 \mathbb{I}_2 \end{pmatrix}$$

with eigenvalues

$$\mu_1(p) = \mu_2(p) = -\mu_3(p) = -\mu_4(p) = \sqrt{c^2|p|^2 + c^4 m^2} \equiv \mu(p).$$

The unitary transformation which diagonalize $\hat{D}(p)$ is given by

$$U(p) = a_+(p)\mathbb{I} + a_-(p)\boldsymbol{\beta}\,\frac{\underline{\boldsymbol{\alpha}} \cdot p}{|p|}\,; \quad a_\pm(p) = \sqrt{\frac{1}{2}\left(1 \pm \frac{mc^2}{\mu(p)}\right)}.$$

We have

$$U(p)\hat{D}(p)U^{-1}(p) = \mu(p)\boldsymbol{\beta} = \sqrt{c^2|p|^2 + m^2 c^4}\begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}.$$

D_0 is *essentially self-adjoint* and self-adjoint on $\mathcal{D}(D_0) = H^1(\mathbb{R}^3, \mathbb{C}^4)$ with purely absolutely continuous spectrum

$$\sigma(D_0) = (-\infty, -mc^2] \cup [mc^2, +\infty).$$

There are two infinite rank orthogonal projectors on $L^2(\mathbb{R}^3, \mathbb{C}^4)$,

$$\Lambda_\pm = \mathcal{F}^{-1} U(p)^{-1} \left(\frac{\mathbb{I}_4 \pm \boldsymbol{\beta}}{2} \right) U(p) \mathcal{F}$$

such that

$$D_0 \Lambda_\pm = \Lambda_\pm D_0 = \pm\sqrt{-c^2\Delta + m^2 c^4}\, \Lambda_\pm$$
$$= \pm\Lambda_\pm \sqrt{-c^2\Delta + m^2 c^4}$$

and, denoting $\mathcal{H}_+ = \Lambda_\pm L^2(\mathbb{R}^3, \mathbb{C}^4)$ *the positive/negative energies subspaces, we have* $L^2(\mathbb{R}^3, \mathbb{C}^4) = \mathcal{H}_+ \oplus \mathcal{H}_-$.

The Foldy-Wouthuysen (unitary) transformation

$$U_{\text{FW}} = \mathcal{F}^{-1} U(p) \mathcal{F}$$

$$\Rightarrow \qquad \Lambda_{\pm,FW} = U_{\text{FW}} \Lambda_{\pm} U_{\text{FW}}^{-1} = \frac{\mathbb{I}_4 \pm \beta}{2}$$

Let denote $\phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^2 \times \mathbb{C}^2)$ we have

positive energy $\Rightarrow$ 2-*upper* components $\psi_+ = U_{\text{FW}}^{-1} \begin{pmatrix} \phi_+ \\ 0 \end{pmatrix} \in \mathcal{H}_+$

negative energy $\Rightarrow$ 2-*lower* components $\psi_- = U_{\text{FW}}^{-1} \begin{pmatrix} 0 \\ \phi_- \end{pmatrix} \in \mathcal{H}_-$

$$D_{\text{FW}} = U_{\text{FW}} D_0 U_{\text{FW}}^{-1} = \sqrt{-c^2 \Delta + m^2 c^4}\, \beta$$

[see B.Thaller, *The Dirac equation*, Springer-Verlag, (1992)] The operator $\sqrt{-c^2\Delta + m^2c^4}$ is related to the Dirichlet problem:

$$\begin{cases} (-\partial_x^2 - c^2\Delta_y + m^2c^4)\phi = 0 & \text{in } \mathbb{R}^4_+ = \{\,(x,y) \in \mathbb{R}\times\mathbb{R}^3 \mid x > 0\,\} \\ \phi(0,y) = \xi(y) \in \mathcal{S}(\mathbb{R}^3) & \text{for } y \in \mathbb{R}^3 = \partial\mathbb{R}^4_+. \end{cases}$$

Indeed, solving the equation via partial Fourier transform we get

$$\phi(x,y) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ip\cdot y}\hat{\xi}(p) e^{-x\sqrt{c^2|p|^2+m^2c^4}}\, dp.$$

We define *the Dirichlet to Neumann operator* $\mathcal{T}_{DN}$ as follows

$$\begin{aligned} \mathcal{T}_{DN}\xi(y) &= \frac{\partial\phi}{\partial\nu}_{|_{\partial\mathbb{R}^4_+}}(y) = -\frac{\partial\phi}{\partial x}(0,y) \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ip\cdot y} \sqrt{c^2|p|^2 + m^2c^4}\, \hat{\xi}(p)\, dp, \end{aligned}$$

namely $\mathcal{T}_{DN} = \sqrt{-c^2\Delta_y + m^2c^4}$ on the dense domain $\mathcal{S}(\mathbb{R}^3)$.

Notation:

$$H^{1/2} \equiv H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \text{ or } H^{1/2}(\mathbb{R}^3, \mathbb{C}^2), \qquad H^1 \equiv H^1(\mathbb{R}^4_+, \mathbb{C}^4) \text{ or } H^1(\mathbb{R}^4_+, \mathbb{C}^2)$$

$$\|\phi\|^2_{H^1} = \iint_{\mathbb{R}^4_+} (|\partial_x \phi|^2 + c^2 |\nabla_y \phi|^2 + m^2 c^4 |\phi|^2)\, dx\, dy$$

$$|\xi|^2_{H^{1/2}} = \int_{\mathbb{R}^3} \sqrt{c^2|p|^2 + m^2 c^4}\, |\hat{\xi}|^2\, dp.$$

Let $\xi \in H^{1/2}$, define the *extension of ξ on the half-space $\mathbb{R}^4_+$*

$$\phi(x,y) = \mathcal{F}_y^{-1}\left(\hat{\xi}(p) e^{-x\sqrt{c^2|p|^2 + m^2 c^4}}\right) \tag{1}$$

then $\phi \in H^1$ and

$$|\xi|_{H^{1/2}} = \|\phi\|_{H^1} = \inf\{\|w\|_{H^1} \;:\; w_{\mathrm{tr}} = \xi\}$$

$$mc^2 \int_{\mathbb{R}^3} |\xi|^2\, dy \leq \inf_{w_{\mathrm{tr}} = \xi} \iint_{\mathbb{R}^4_+} (|\partial_x w|^2 + m^2 c^4 |w|^2)\, dx\, dy.$$

Perturbed Dirac operators

We are interested in the perturbed Dirac operators $D_0 + V$, $V \in L^3_w(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ being a scalar potential.

$L^q_w(\mathbb{R}^N)$ denotes the weak L^q space, the space of all measurable functions f such that

$$\sup_{\mu>0} \mu\,|\{x\,:\,|f(x)|>\mu\}|^{1/q} < +\infty,$$

where $|\cdot|$ denotes the Lebesgue measure, or equivalently, for $\frac{1}{q}+\frac{1}{r}=1$

$$\|f\|_{q,w} = \sup_A |A|^{-1/r}\int_A |f(x)| < +\infty.$$

The Coulomb potential $V(x) = -\frac{e^2 Z}{|x|}$ in $L^3_w(\mathbb{R}^3)$.

Let define the sesquilinear form $\mathcal{E} : H^{1/2} \times H^{1/2} \to \mathbb{C}$ as follows

$$\mathcal{E}(f,g) = \int_{\mathbb{R}^3} (\hat{f}(p), (c\underline{\alpha}\cdot p + mc^2\beta)\hat{g}(p))_{\mathbb{C}^4}\, dp + \int_{\mathbb{R}^3} V(x)(f,g)_{\mathbb{C}^4}\, dx$$

We look for solutions $(\psi, \lambda) \in H^{1/2} \times \mathbb{R}$ of the (weak) equation

$$\mathcal{E}(\psi, h) = \lambda \langle \psi | h \rangle_{L^2}, \qquad \forall h \in H^{1/2}.$$

Equivalently, setting $\xi = U_{\mathrm{FW}} \psi$, we look for solutions $(\xi, \lambda) \in H^{1/2} \times \mathbb{R}$ of the (weak) equation

$$\mathcal{E}_{\mathrm{FW}}(\xi, h) = \lambda \langle \xi | h \rangle_{L^2}, \qquad \forall h \in H^{1/2}, \tag{2}$$

where

$$\mathcal{E}_{\mathrm{FW}}(\xi, h) = \int_{\mathbb{R}^3} \sqrt{c^2 |p|^2 + m^2 c^4}\ (\hat{\xi}(p), \beta \hat{h}(p))_{\mathbb{C}^4}\, dp + \int_{\mathbb{R}^3} V(x) (U_{\mathrm{FW}}^{-1} \xi, U_{\mathrm{FW}}^{-1} h)_{\mathbb{C}^4}\, dx.$$

The extension on $\mathbb{R}^4_+$: the Dirichlet to Neumann operator

Let $(\xi_\lambda, \lambda) \in H^{1/2} \times \mathbb{R}$ be a solution of (2) and let ϕ_λ be the *extension* of ξ_λ on the half-space $\mathbb{R}^4_+$ then $\phi_\lambda \in H^1(\mathbb{R}^4_+, \mathbb{C}^4)$, $(\phi_\lambda)_{tr} = \xi_\lambda$ and (ϕ_λ, λ) is a solution of *the Neumann problem*

$$\begin{cases} (-\partial_x^2 - c^2\Delta_y + m^2c^4)\phi_\lambda = 0 & \text{in } \mathbb{R}^4_+ \\ \beta \dfrac{\partial \phi_\lambda}{\partial \nu}_{|_{\partial\mathbb{R}^4_+}} = -U_{FW} V U_{FW}^{-1} \xi_\lambda + \lambda \xi_\lambda & \text{on } \partial\mathbb{R}^4_+ = \mathbb{R}^3. \end{cases} \qquad (\mathcal{E}_\lambda)$$

On the other hand, if $(\phi_\lambda, \lambda) \in H^1 \times \mathbb{R}$ solves *the Neumann problem* $(\mathcal{E}_\lambda)$, setting $\xi_\lambda = (\phi_\lambda)_{tr}$ the *trace* of ϕ_λ, then $(\xi_\lambda, \lambda) \in H^{1/2}$ is a solution of (2).

[L. Caffarelli; L. Silvestre, *An extension problem related to the fractional Laplacian*, Comm. PDE (2007)]

Variational setting

We consider the functional

$$\mathcal{I}(\phi) = \|\phi_+\|^2_{H^1} - \|\phi_-\|^2_{H^1} + \int_{\mathbb{R}^3} V(y)(U_{\mathrm{FW}}^{-1}\phi_{tr}, U_{\mathrm{FW}}^{-1}\phi_{tr})_{\mathbb{C}^4}\, dy$$

where $\phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} \in H^1$ and $\phi_{tr} \in H^{1/2}$.

Then $(\phi_\lambda, \lambda) \in H^1 \times \mathbb{R}$ is a (weak) solution of the *Neumann problem* $(\mathcal{E}_\lambda)$ if and only if

$$d\mathcal{I}(\phi_\lambda)[h] = \lambda\, 2\,\mathrm{Re}\, \langle (\phi_\lambda)_{tr} | h_{tr} \rangle_{L^2} \qquad \forall h \in H^1.$$

- Projected Dirac operator: *the Brown-Ravenhall Hamiltonian*

  see S. Morozov S. Vugalter *Ann. H. Poincaré (2006)* for related pb.; V. Coti Zelati; M.N. *NLA (2016)*,

- *Pohozaev identity* ⇒ *Relativistic virial theorem*

  see e.g. B.Thaller, *The Dirac equation*, Springer-Verlag, (1992) ; V. Coti Zelati ; M.N. *JFPT (2017)*

- *Variational characterizations for the (positive) eigenvalues for*
  - *the Dirac-Coulomb problem*

    (see J. Dolbeaut, M. Esteban, E. Séré *Calc.Var. PDE (2000))*
  - *the Maxwell-Dirac -Coulomb problem*

    V. Coti Zelati ; M.N. *in progress*

The Maxwell-Dirac-Coulomb system

The MDC system describes an electron interacting with its own electromagnetic field (*extended particle* : $\Psi(t,x) = e^{-i\lambda t}\psi(x)$) and with a nucleus of atomic number Z

$$(\mathcal{P})_{MDC} \begin{cases} -ic\underline{\alpha}\cdot(\nabla - i\frac{e}{c}\underline{A})\psi + mc^2\beta\psi + e\Phi\psi + V_Z\psi = \lambda\psi \\ -\Delta\Phi = 4\pi\rho\,; \qquad -\Delta\underline{A} = \frac{4\pi}{c}\underline{J} \\ |\psi|^2_{L^2} = 1 \end{cases}$$

where $V_Z = -\frac{Ze^2}{|x|}$, $e = -|e|$ is the electron charge and $(c\rho, \underline{J})$ is the *Dirac relativistic current* $(c\partial_t\rho + \nabla\cdot\underline{J} = 0)$, given by

$$\rho = e|\psi|^2 \qquad \underline{J} = e(\psi, c\underline{\alpha}\psi)$$

hence by the Poisson formula we get

$$\Rightarrow \begin{cases} \Phi = \rho * \frac{1}{|x|} = e|\psi|^2 * \frac{1}{|x|} \\ \underline{A} = \frac{1}{c}\underline{J} * \frac{1}{|x|} = e(\psi, \underline{\alpha}\psi) * \frac{1}{|x|} \end{cases}$$

(see G.M. Coclide, V. Georgiev *JDE(2004))* for the Maxwell-Schrödinger-Coulomb eq. ;
see M.Esteban, V. Georgiev, E. Sèrè *Calc.Var. PDE (1996)*) for stationary solutions of the Maxwell-Dirac eq.)

The MDC (nonlinear) eigenvalues problem

We look for solutions $(\psi, \lambda) \in H^{1/2} \times \mathbb{R}$ of the nonlinear equation

$$(\mathcal{P})_{MDC} \Rightarrow \begin{cases} D_0\psi + W_{int}\psi = \lambda\psi \\ |\psi|^2_{L^2} = 1 \end{cases}$$

where the *effective potential* $W_{int} \equiv V_z + e\Phi - e\underline{A} \cdot \underline{\alpha} \in L^3_w(\mathbb{R}^3)$, indeed $|\underline{A}| \leq \Phi$ and if $\psi \in L^2$ then $\Phi \in L^3_w(\mathbb{R}^3)$.

In the FW representation we look for (weak) solutions $(\phi, \lambda) \in H^1 \times \mathbb{R}$ of the *nonlinear Neumann problem*

$$(\mathcal{E}_\lambda) \begin{cases} (-\partial_x^2 - c^2\Delta_y + m^2c^4)\phi = 0 & \text{in } \mathbb{R}^4_+ \\ \beta \frac{\partial \phi}{\partial \nu}_{|_{\partial\mathbb{R}^4_+}} + U_{\text{FW}}(V_z + e\Phi - e\underline{\alpha} \cdot \underline{A})U^{-1}_{\text{FW}}\phi_{tr} = \lambda\phi_{tr} & \text{on } \partial\mathbb{R}^4_+ \\ |\phi_{tr}|^2_{L^2} = 1 \\ \Phi = e|U^{-1}_{\text{FW}}\phi_{tr}|^2 * \frac{1}{|x|}; \quad \underline{A} = e(U^{-1}_{\text{FW}}\phi_{tr}, \underline{\alpha}U^{-1}_{\text{FW}}\phi_{tr}) * \frac{1}{|x|} \end{cases}$$

Variational setting

We consider the functional $\mathcal{I}(\phi)$ on H^1, $\phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} \in X_+ + X_-$

$$\mathcal{I}(\phi) = \|\phi_+\|^2_{H^1} - \|\phi_-\|^2_{H^1} \; - Ze^2 \int_{\mathbb{R}^3} \frac{\rho_\phi(y)}{|y|}\, dy + \frac{e^2}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\phi(y)\rho_\phi(z) - J_\phi(y) \cdot J_\phi(z)}{|y-z|}\, dy\, dz$$

where $\rho_\phi = |U_{\mathrm{FW}}^{-1}\phi_{tr}|^2$ and $J_\phi = (U_{\mathrm{FW}}^{-1}\phi_{tr}, \underline{\alpha} U_{\mathrm{FW}}^{-1}\phi_{tr})$.

$(\phi_\lambda, \lambda) \in H^1 \times \mathbb{R}$ is a (weak) solution of the *Neumann nonlinear problem* $(\mathcal{E}_\lambda)$ if and only if

$$d\mathcal{I}(\phi_\lambda)[h] = \lambda\, 2\, \mathrm{Re}\, \langle (\phi_\lambda)_{tr} | h_{tr} \rangle_{L^2} \qquad \forall h \in H^1.$$

Existence of the "Ground state"

Given $W \subset X_+$ a 1-dim vector space, let define

$$\mathcal{X}_W = \{\phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} \in W \oplus X_- \, : \, |\phi_{tr}|_{L^2} = 1\}.$$

Then we define

$$\lambda_1 = \inf_{\substack{W \subset X_+ \\ dim W = 1}} \sup_{\phi \in \mathcal{X}_W} \mathcal{I}(\phi)$$

Theorem (*"ground state"*)
If the atomic number $Z < 124$ then

- $\lambda_1 \in (0, mc^2)$
- *there exists* $\phi_{\lambda_1} \in H^1$ *, such that* $|(\phi_{\lambda_1})_{tr}|_{L^2} = 1$ *and*

$$d\mathcal{I}(\phi_{\lambda_1})[h] = \lambda_1 \, 2 \, \mathrm{Re} \, \langle (\phi_{\lambda_1})_{tr} | h_{tr} \rangle_{L^2} \qquad \forall h \in H^1.$$

Let us recall some important inequalities

- *Kato inequality:* For any $\psi \in H^{1/2}$

$$\langle \psi | |x|^{-1} \psi \rangle_{L^2} \leq \frac{\pi}{2} \langle \psi | \sqrt{-\Delta} \psi \rangle_{L^2} \leq \frac{\pi}{2c} \langle \psi | \sqrt{-c^2\Delta + m^2 c^4} \psi \rangle_{L^2}$$

- *Tix inequality** for any $\psi \in H^{1/2}$

$$\langle \Lambda_\pm \psi | |x|^{-1} \Lambda_\pm \psi \rangle_{L^2} \leq \frac{1}{2c} \left(\frac{\pi}{2} + \frac{2}{\pi} \right) \langle \Lambda_\pm \psi | \sqrt{-c^2\Delta + m^2 c^4} \Lambda_\pm \psi \rangle_{L^2}$$

Note that if $Z < Z_c = 124$ then $\frac{Ze^2}{c} \left(\frac{\pi}{2} + \frac{2}{\pi} \right) < 1$, hence the positive/negative energy components the Coulomb potential term are $H^{1/2}$- bounded. Recall that the Dirac – Coulomb operator is essentially self-adjoint if $Z < 118$ ([Schmincke ('72)]).

Lemma Let $\rho \in L^1(\mathbb{R}^3)$ and $\psi \in H^{1/2}$

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(x) |\psi|^2(y)}{|x - y|} \leq \frac{\pi}{2c} |\rho|_{L^1} |\psi|^2_{H^{1/2}}.$$

* C. Tix, *Strict positivity of a relativistic Hamiltonian due to Brown and Ravenhall*, Bull. Lon. Math. Soc. (1998)

Sketch of the proof

step 1 For any $W \subset X_+$, $dim W = 1$, there exists $\phi_w \in \mathcal{X}_W$ such that

$$\lambda_w = \sup_{\phi \in \mathcal{X}_W} \mathcal{I}(\phi) = \mathcal{I}(\phi_w) > 0$$

For any $\eta > 0$ let define the auxiliary problems

$$\lambda_w(\eta) = \sup\{\mathcal{I}(\phi) \,|\, \phi \in W \oplus X_-; \quad |\phi_{tr}|^2_{L^2} = \eta\}$$

- $\lambda_w(\eta) > 0$ (no vanishing);
- $\lambda_w > \lambda_w(1-\delta) + \lambda_w(\delta)$ for any $\delta \in (0,1)$ (no dicothomy).

$$\Rightarrow \quad d\mathcal{I}(\phi_w)[h] = \lambda_w 2\,\mathrm{Re}\langle(\phi_w)_{tr}|h_{tr}\rangle_{L^2} \qquad \forall\ h \in W \oplus X_-$$

step 2 Take $v \in \mathbb{C}_0^\infty(\mathbb{R}^3)$ *non-negative, radially symmetric and non-increasing* . Let $W_\eta = \text{span}\{w_\eta\}$ where

$$w_\eta(x,y) = e^{-mc^2 x}\eta^{3/2}\begin{pmatrix} v(\eta y) \\ 0 \end{pmatrix}$$

$$\exists \bar\eta > 0 : \quad \sup_{\phi \in \mathcal{X}_{W_{\bar\eta}}} \mathcal{I}(\phi) < mc^2 \ \Rightarrow \ 0 < \lambda_1 < mc^2$$

- $\|w_\eta\|_{H^1}^2 - mc^2|v|_{L^2}^2 = \eta^2 \dfrac{1}{2m}|\nabla v|_{L^2}^2$
- $\displaystyle\int_{\mathbb{R}^3} \frac{\rho_{\phi_\eta}(y)}{|y|} = \eta a^2 \int_{\mathbb{R}^3} \frac{|v|^2}{|y|} + \int_{\mathbb{R}^3} \frac{\rho_{\phi_2}}{|y|} + O(\eta^2)$
- $\displaystyle\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{\phi_\eta}(y)\rho_{\phi_\eta}(z)}{|y-z|} = \eta a^2 |\rho_{\phi_\eta}|_{L^1} \int_{\mathbb{R}^3} \frac{|v|^2}{|y|}$
  $\displaystyle + \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{\phi_\eta}(y)\rho_{\phi_2}(z)}{|y-z|} + \cdots + O(\eta^2)$

$$\Rightarrow \mathcal{I}(\phi_\eta) - mc^2 \le \eta^2 a^2 \frac{1}{2m}|\nabla v|_{L^2}^2 - \frac{1}{2}\,\|\phi_2\|_{H^1}^2$$
$$- \eta \frac{1}{2} a^2 e^2 (2Z-1) \int_{\mathbb{R}^3} \frac{|v_0|^2}{|y|}$$
$$- mc^2 |(\phi_2)_{tr}|_{L^2}^2 + O(\eta^2)$$

step 3 Take $W_n \subset X_+$ a *minimizing sequence*:

$$\sup_{\phi \in \mathcal{X}_{W_n}} \mathcal{I}(\phi) = \mathcal{I}(\phi_n) = \lambda_{W_n} \to \lambda_1$$

$$\Rightarrow \begin{cases} T_n(h) = d\mathcal{I}(\phi_n)[h] - \lambda_{W_n} 2\,\mathrm{Re}\langle (\phi_n)_{tr} | h_{tr} \rangle_{L^2} \quad (\forall h \in H^1) \\ T_n(h) = 0; \quad \forall h \in W_n \oplus X_- \\ |(\phi_n)_{tr}|_{L^2}^2 = 1; \qquad \phi_{+,n} \neq 0 \qquad (\forall n \in \mathbb{N}). \end{cases}$$

- The sequence (ϕ_n) is bounded in H^1

Take $h_n = \begin{pmatrix} \phi_{+,n} \\ -\phi_{-,n} \end{pmatrix} \in W_n \oplus X_-$ we have

$$\begin{aligned}
2\lambda_{1,n} \geq & \lambda_{1,n} 2\,\mathrm{Re}\langle (\phi_n)_{tr}, (h_n)_{tr}\rangle_{L^2} = d\mathcal{I}(\phi_n)[h_n] \\
\geq & 2\|\phi_{+,n}\|^2_{H^1} - 2Ze^2 \int_{\mathbb{R}^3} \frac{\rho_{\phi_{+,n}}}{|y|} \\
& \quad + 2\|\phi_{2,n}\|^2_{H^1} - 4e^2 \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{\phi_n}(y)\rho_{\phi_{-,n}}(z)}{|y-z|}\, dy\, dz \\
\geq & 2(1-\gamma_1)\|\phi_{1,n}\|^2_{H^1} + 2(1-\gamma_2)\|\phi_{2,n}\|^2_{H^1}
\end{aligned}$$

where $\gamma_1 = \frac{Ze^2}{c}\frac{1}{2}(\frac{\pi}{2} + \frac{2}{\pi}) < 1$ (whenever $Z < 124$) and $\gamma_2 = \pi\frac{e^2}{c} < 1/43$.

- $T_n \to 0$ in H^{-1}

If not $\exists \chi_n = \binom{\chi_{1,n}}{0} \in (W_n \oplus X_-)^\perp \subset X_+$, $T_n(\chi_n) \geq \delta > 0$.
Let $W_t = \mathrm{span}\{\phi_{+,n} - t\chi_{1,n}\}$ we get for $t > 0$ sufficiently small

$$\sup_{\phi \in \mathcal{X}_{W_t}} \mathcal{I}(\phi) \leq \cdots \leq \lambda_{1,n} - t\frac{\delta}{4} < \lambda_1.$$

a contradiction.

$$\Rightarrow \sup_{h \in H^1 : \|h\|_{H^1} = 1} |d\mathcal{I}(\phi_n)[h] - \lambda_{W_n} 2\,\mathrm{Re}\langle (\phi_n)_{tr} | h_{tr} \rangle_{L^2}| = o(1)$$

step 4 Let $v_n = \phi_n - \bar{\phi} \rightharpoonup 0$ then $(v_n)_{tr} \to 0$ strongly in L^2.

$$\Rightarrow \begin{cases} d\mathcal{I}(\bar{\phi})[h] = \lambda_1 2\,\mathrm{Re}\langle \bar{\phi}_{tr} | h_{tr} \rangle_{L^2} & \forall\, h \in H^1 \\ |\bar{\phi}_{tr}|^2_{L^2} = 1 \end{cases}$$

- $\int_{\mathbb{R}^3} \frac{\rho_{v_{+,n}}}{|y|} \to 0$

Take $h_{R,n} = \theta_R^2(y) \begin{pmatrix} v_{+,n} \\ -v_{-,n} \end{pmatrix}$ where θ_R is a cut-off function.

$$\begin{aligned}
o_n(1) =& T_n(h_{R,n}) = d\mathcal{I}(\phi_n)[h_{R,n}] - 2\lambda_{1,n} \operatorname{Re}\langle(\phi_n)_{tr}|(h_{R,n})_{tr}\rangle_{L^2} \\
\geq& 2\|\theta_R v_{+,n}\|_{H^1}^2 + 2\|\theta_R v_{-,n}\|_{H^1}^2 + o_R(1) \\
&- 2Ze^2 \int_{\mathbb{R}^3} \frac{\rho_{\theta_R v_{+,n}}}{|y|} + 2Ze^2 \int_{\mathbb{R}^3} \frac{\rho_{\theta_R v_{-,n}}}{|y|} \\
&- C\|[U_{\mathrm{FW}}^{-1}, \theta_R]\| \, |(v_n)_{tr}|_{H^{1/2}}^2 + o_n(1) \\
\geq& 2(1-\gamma)\|\theta_R v_{+,n}\|_{H^1}^2 + o_n(1) + o_R(1)
\end{aligned}$$

since $\|[U_{\mathrm{FW}}^{-1}, \theta_R]\| = o_R(1)$ and

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{\phi_n}(y) \operatorname{Re}(U_{\mathrm{FW}}^{-1}(\phi_n)_{tr}, U_{\mathrm{FW}}^{-1}(h_{R,n})_{tr})|(z)}{|y-z|} \, dy \, dz = o_n(1)$$

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{J_{\phi_n}(y) \operatorname{Re}(U_{\mathrm{FW}}^{-1}(\phi_n)_{tr}, \underline{\alpha} U_{\mathrm{FW}}^{-1}(h_{R,n})_{tr})(z)}{|y-z|} \, dy \, dz = o_n(1)$$

- $\phi_n \to \bar{\phi}$ strongly in H^1 hence in particular $|\bar{\phi}_{tr}|^2_{L^2} = 1$

Take $h_n = \binom{v_{+,n}}{-v_{-,n}}$, since $mc^2 > \lambda_1$, we get

$$
\begin{aligned}
o(1) =& T_n(h_n) = d\mathcal{I}(\phi_n)[h_n] - \lambda_{1,n} 2\,\mathrm{Re}\langle(\phi_n)_{tr}|(h_n)_{tr}\rangle_{L^2} \\
&\geq 2\|v_{+,n}\|^2_{H^1} + 2\|v_{-,n}\|^2_{H^1} - 2Ze^2 \int_{\mathbb{R}^3} \frac{\rho_{v_{+,n}}}{|y|} \\
&- 4e^2 \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{\phi_n}(y)\rho_{v_{-,n}}(z)}{|y-z|}\,dy\,dz \\
&- 2\lambda_{1,n}|(v_{+,n})_{tr}|^2_{L^2} + o(1) \\
\geq& 2\left(1 - \frac{\lambda_{1,n}}{mc^2}\right)\|v_{+,n}\|^2_{H^1} + 2(1-\gamma_2)\|v_{-,n}\|^2_{H^1} + o(1)
\end{aligned}
$$

The Virial Theorem for Dirac Equation

The *Virial Theorem* for the (perturbed) Dirac operator $D_0 + V$ states that if ψ is an eigenfunction then

$$\langle \psi | - ic\underline{\boldsymbol{\alpha}} \cdot \nabla \psi \rangle = \langle \psi | x \cdot \nabla V \psi \rangle$$

This identity has been proved by Albeverio ('72), Kalf ('76) and refined by Leinfelder ('81).
The Virial Theorem can be used to prove that there is no eigenvalue for H in the essential spectrum.

We give an alternative proof of the the Virial Theorem under the same assumptions given by Leinfelder (1981). The proof is based in a *Pohozaev-like identity* for $(\mathcal{E}_\lambda)$, the Neumann problem in $\mathbb{R}^4_+$.

Assumptions on V:

(h1) $V \in L^3_w(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ such that

(i) there exists, for almost all $x \in \mathbb{R}^3$, the limit

$$\lim_{\theta \to 1} \frac{V(\theta x) - V(x)}{\theta - 1} = |x| \partial_r V(x);$$

(ii) there exists $f \in L^3_w(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and $\delta > 0$ such that for $|\theta - 1| < \delta$

$$\frac{|V(\theta x) - V(x)|}{|\theta - 1|} \leq f(x) \qquad \text{a.e.}.$$

Let us point out that if V is sufficiently regular

$$\lim_{\theta \to 1} \frac{V(\theta x) - V(x)}{\theta - 1} = |x| \partial_r V(x) = (x, \nabla V(x)).$$

and (ii) is slightly more general then

$$\frac{|V(\theta x) - V(x)|}{|\theta - 1|} \leq \frac{c_1}{|x|} + c_2,$$

for some $c_1, c_2 > 0$, the assumption one finds in Kalf (1976) and Thaller (1992).

Theorem (*Pohozaev-like identity*)
Let (**h1**) holds and let $\phi_\lambda \in H^1(\mathbb{R}^4_+, \mathbb{C}^4)$ be a weak solution of $(\mathcal{E}_\lambda)$ then setting $(\phi_\lambda)_{tr} = \xi_\lambda$ and $\psi_\lambda = U_{\mathrm{FW}}^{-1}\xi_\lambda$ we have

$$\int_{\mathbb{R}^3} (|x|\partial_r V)|\psi_\lambda|^2\, dx = \int_{\mathbb{R}^3} (\hat{\psi}_\lambda, c\,\underline{\alpha} \cdot p\,\hat{\psi}_\lambda)\, dp.$$

or, equivalently

$$\lambda = \int_{\mathbb{R}^3} (|x|\partial_r V + V)|\psi_\lambda|^2\, dx + \langle \psi_\lambda, \beta mc^2 \psi_\lambda \rangle_{L^2}$$

Sketch of the proof

Let $\phi_\lambda \in H^1$ be a (weak) solution of the Neumann problem $(\mathcal{E}_\lambda)$, we have

$$d\mathcal{I}(\phi_\lambda)[h] = \lambda\, 2\,\mathrm{Re}\, \langle (\phi_\lambda)_{tr} | h_{tr} \rangle_{L^2} \qquad \forall h \in H^1.$$

Take

$$h = U_{\mathrm{FW}} \mathcal{D}_y^\theta U_{\mathrm{FW}}^{-1} \phi_\lambda \in H^1$$

where $\mathcal{D}_y^\theta = \frac{1}{2}(D_y^\theta + D_y^{1/\theta})$ and for $0 < \theta \neq 1$

$$D_y^\theta f(x,y) = \theta^2 \frac{f(x,\theta y) - f(x,y)}{\theta - 1}.$$

If f is sufficiently regular we have that

$$\lim_{\theta \to 1} D_y^\theta f(x,y) = \lim_{\theta \to 1} \theta^2 \frac{f(x,\theta y) - f(x,y)}{\theta - 1} = (y, \nabla_y f).$$

After some computations, same estimate and passing to the limit as $\theta \to 1$ one obtains the result.

To relate the above result with the eigenvalue problem for Dirac operator and the corresponding (relativistic) Virial Theorem we need an *additional assumption*

(h2) $D_0 + V$ has a self-adjoint extension H which is the unique such that its domain $\mathcal{D}(H)$ is contained in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and the corresponding form defined in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ satisfies $\forall f \in \mathcal{D}(H)$ and $\forall g \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$:

$$\langle Hf, g\rangle = \mathcal{Q}_{D_0}(f, g) + \mathcal{Q}_V(f, g)$$

If **(h2)** holds then any eigenfunction ψ_λ of H with eigenvalue λ satisfies

$$\langle H\psi_\lambda, h\rangle = \mathcal{E}(\psi_\lambda, h) = \lambda\langle\psi_\lambda|h\rangle, \qquad \forall h \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4).$$

Letting $\xi_\lambda = U_{\text{FW}}\psi_\lambda$, the extension on the half-space of ξ_λ is a weak solution of the Neumann boundary value problem $(\mathcal{E}_\lambda)$, hence by the above theorem follows

Theorem. (Relativistic Virial Theorem)

Let (**h1**)*-*(**h2**) *hold. Let* $\psi_\lambda \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^4)$ *be an eigenfunction of* H*, with corresponding eigenvalue* $\lambda \in \mathbb{R}$*. Then*

$$\int_{\mathbb{R}^3} (|x|\partial_r V)|\psi_\lambda|^2\, dx = \int_{\mathbb{R}^3} (\hat{\psi}_\lambda, c\,\underline{\boldsymbol{\alpha}} \cdot p\, \hat{\psi}_\lambda)\, dp$$

or, equivalently

$$\lambda = \langle H\psi_\lambda, \psi_\lambda\rangle = \int_{\mathbb{R}^3} (|x|\partial_r V + V)|\psi_\lambda|^2\, dx + \langle \psi_\lambda, mc^2\boldsymbol{\beta}\psi_\lambda\rangle_{L^2}.$$

Hence, in particular

- $\lambda \leq mc^2$ *whenever* $|x|\partial_r V(x) + V(x) \leq 0$
- $\lambda \geq -mc^2$ *whenever* $|x|\partial_r V(x) + V(x) \geq 0.$

Remark.

The Dirac-Coulomb operator $D_0 - \gamma|x|^{-1}$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3 \setminus \{0\})$ and self-adjoint in $H^1(\mathbb{R}^3, \mathbb{C}^4)$ for $\gamma < c\sqrt{3}/2$ corresponding to a critical value $Z = 118$. For $c\sqrt{3}/2 \leq \gamma < c$ $(Z = 137)$ there exists a self-adjoint extension H which is *uniquely* characterized by the property that the domain is contained in the D_0-form domain $H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$ and (**??**) holds, see Schmincke (1972) and in particular Nenciu (1976). As a consequence, assumption (**h2**) holds for $D_0 - \frac{\gamma}{|x|}$ when $\gamma \in (0, c)$.

Remark.

The essential spectrum of the free Dirac operator D_0 is given by

$$\sigma_{ess}(D_0) = \sigma(D_0) = (-\infty, -mc^2] \cup [mc^2, +\infty).$$

It is known (see Nenciu (1976)) that for the Dirac Coulomb operator with $\gamma \in (0, c)$

$$\sigma_{ess}(H) \subseteq \sigma_{ess}(D_0)$$

Hence in particular the Virial Theorem implies the absence of eigenvalues in the essential spectrum for the Coulomb potential, since for such a potential

$$|x|V_r(x) + V(x) = (x, \nabla V) + V = 0.$$