Ground state for the relativistic one electron atom

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Variational methods, with applications to problems in mathematical physics and geometry;
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[joint work with Vittorio Coti Zelati – Università di Napoli "Federico II"]

The QED Lagrangian

The *Lagrangian* for a *charged, spin-$\frac{1}{2}$ relativistic particle* is

$$\mathcal{L} = \bar{\Psi}(i\gamma^\mu D_\mu - 1)\Psi - \frac{1}{16\pi} F_{\mu\nu}F^{\mu\nu}$$

here $\hbar = c = m = 1$ and we use the four-vector notations $(\mu = 0, 1, 2, 3)$ $x^\mu = (ct, \underline{x}) \in \mathbb{R}^4$, with metric tensor $g_{\mu\nu} = \mathrm{diag}\{1, -1 - 1, -1\}$ used to lower or raise the Lorentz indices,

- Ψ is the *Dirac spinor* and $\bar{\Psi} = \Psi^\dagger \gamma^0$ is the *Dirac adjoint* ;
- γ^μ are the 4×4 *Dirac matrices* ;
- $D_\mu = \partial_\mu + ie(A_\mu + A_\mu^{ext})$ is the *gauge covariant derivative* ;
- e is the charge (coupling constant);
- A_μ is the *electromagnetic 4-vector potential generated by the electron itself* ;
- $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the *electromagnetic tensor field* ;
- A_μ^{ext} is the *external electromagnetic potential.*

The Euler-Lagrange equations: Maxwell-Dirac system

The *Euler-Lagrange equations* in the *Lorenz gauge:* $\partial_\mu A^\mu = 0$ are given by the following *Maxwell-Dirac system*

$$\begin{cases} (i\gamma^\mu \partial_\mu - 1)\Psi = e\,\gamma^\mu (A_\mu + A_\mu^{ext})\Psi \\ \Box A^\mu = 4\pi\, j^\mu \end{cases}$$

where $j^\mu = e\,\bar{\Psi}\gamma^\mu\Psi$ is the conserved *Dirac current* $\Rightarrow\ \partial_\mu j^\mu = 0$.

- *External source*: (not relativistic) nucleus of atomic number Z

$$A_0^{ext} = \frac{Z|e|}{|x|}; \qquad A_k^{ext} = 0 \quad (k = 1, 2, 3)$$

- *Ground state*: We look for a bound state of *lowest positive energy*, a *stationary solution*

$$\Psi(t, x) = \mathrm{e}^{-iEt}\psi(x); \qquad \textit{with} \quad |\psi|_{L^2} = 1$$

and $E = E_{min} > 0$.

The Maxwell-Dirac eigenvalue problem

We are lead to consider the following *eigenvalue problem*

$$\begin{cases} (-i\underline{\boldsymbol{\alpha}}\cdot\nabla+\boldsymbol{\beta})\psi-\frac{Ze^2}{|x|}\psi+eA_0\psi-e\underline{\boldsymbol{\alpha}}\cdot\underline{A}\,\psi=E\psi \\ -\Delta A_0=4\pi e\,|\psi|^2 \\ -\Delta\underline{A}=4\pi e\,(\psi,\underline{\boldsymbol{\alpha}}\psi)_{\mathbb{C}^4} \\ |\psi|_{L^2}=1. \end{cases}$$

here $\boldsymbol{\beta}=\gamma^0$, $\underline{\boldsymbol{\alpha}}=\gamma^0(\gamma^1,\gamma^2,\gamma^3)$ are hermitian, unitary matrices,

$$\Rightarrow\ \begin{cases} A_0=e\,|\psi|^2*\frac{1}{|x|} \\ \underline{A}=e\,(\psi,\underline{\boldsymbol{\alpha}}\psi)_{\mathbb{C}^4}*\frac{1}{|x|}. \end{cases}$$

The nonlinear eigenvalue problem

The problem reduces to the *nonlinear* eigenvalue problem:

$$(P)\ \begin{cases} (H_D + V_{ext})\psi + V_{int}(\psi)\psi = E\psi \\ |\psi|_{L^2} = 1 \end{cases}$$

here $H_D = -i\underline{\boldsymbol{\alpha}} \cdot \nabla + \boldsymbol{\beta}$ is the is the (free) *Dirac operator*,

$V_{ext} = -\frac{Ze^2}{|x|}\mathbb{I}_4$ is the *Coulomb potential*, and

$$V_{int}(\psi) = e^2|\psi|^2 * \frac{1}{|x|}\mathbb{I}_4 - e^2\underline{\boldsymbol{\alpha}} \cdot (\psi, \underline{\boldsymbol{\alpha}}\psi)_{\mathbb{C}^4} * \frac{1}{|x|}$$

is the *nonlinear* term, note that $|(\psi, \underline{\boldsymbol{\alpha}}\psi)_{\mathbb{C}^4}|(x) \leq |\psi|^2(x)$.

The free Dirac operator

The (free) Dirac operator $H_D = -i\underline{\alpha}\cdot\nabla + \beta$ is a first order, self-adjoint operator on $H^1(\mathbb{R}^3;\mathbb{C}^4)$ with *purely absolutely continuous* spectrum given by $\sigma(H_D) = (-\infty,-1]\cup[1,+\infty)$.
In *Fourier space* H_D becomes a multiplication operator with eigenvalues $\{\pm\sqrt{|p|^2+1}\}$.

Let $\Lambda_\pm$ the two infinite rank orthogonal projectors on the positive/negative energies subspaces, then

$$H_D\Lambda_\pm = \Lambda_\pm H_D = \pm\sqrt{-\Delta+1}\,\Lambda_\pm = \pm\Lambda_\pm\sqrt{-\Delta+1}.$$

For any $\psi,\phi \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^4)$ the Dirac- operator form is given by

$$\langle\psi|H_D\phi\rangle = \langle\Lambda_+\psi,\Lambda_+\phi\rangle_{H^{1/2}} - \langle\Lambda_-\psi,\Lambda_-\phi\rangle_{H^{1/2}}$$

and we denote $X_\pm = \Lambda_\pm H^{1/2}(\mathbb{R}^3;\mathbb{C}^4)$.

Some useful estimates:

For all $\psi \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$

- $\int_{\mathbb{R}^3} \frac{|\psi|^2}{|x|}\, dx \leq \frac{\pi}{2} |(-\Delta)^{1/4}\psi|^2_{L^2} \leq \frac{\pi}{2} \|\psi\|^2_{H^{1/2}}$ [Kato]

- $\int_{\mathbb{R}^3} \frac{|\Lambda_\pm \psi|^2}{|x|}\, dx \leq \gamma_T \|\Lambda_\pm \psi\|^2_{H^{1/2}}$ [Tix]

  with $\gamma_T = \frac{1}{2}(\frac{\pi}{2} + \frac{2}{\pi}) < \frac{\pi}{2}$, and $Ze^2\gamma_T < 1$ for $Z \leq 124$.

Theorem. (Coti Zelati - N. ; *SIMA (2019)*)

For any $4 < Z < 124$, *there exist* $E_0 \in \mathbb{R}_+ \setminus \sigma(H_D)$ *and* $\psi_0 \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$ *a (weak) solution of*

$$(P) \begin{cases} (H_D + V_{ext})\psi + V_{int}(\psi)\psi = E\psi \\ |\psi|_{L^2} = 1. \end{cases}$$

The lowest positive critical value of the energy functional

$$\mathcal{E}(\psi) = \langle \psi | (H_D + V_{ext})\psi \rangle + \frac{1}{2} \langle \psi | V_{int}(\psi))\psi \rangle$$

is attained and it is given by

$$\lambda = \inf_{\substack{F \subset X_+ \\ \dim F = 1}} \sup_{\substack{\psi \in F \oplus X_- \\ |\psi|_{L^2} = 1}} \mathcal{E}(\psi) = \mathcal{E}(\psi_0).$$

where $X_\pm = \Lambda_\pm H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$ *are the positive/negative (free) energies subspaces, and* E_0 *is the Lagrange multiplier.*

Related results

- Minimax characterization for the positive eigenvalues in the spectral gap for the Dirac-Coulomb operator $H_D + V_{ext}$:

  [Dolbeaut-Esteban-Sere *Calc.Var. PDE* (2000); Morozov-Muller *Math.Z.* (2015) ; .....]

$$\lambda_k = \inf_{\substack{F \subset X_+ \\ dim F = k}} \sup_{\substack{\psi \in F \oplus X_- \\ |\psi|_{L^2} = 1}} \langle \psi | (H_D + V_{ext}) \psi \rangle \qquad k \in \mathbb{N}$$

$\Longrightarrow \lambda_k \in \sigma_{disc} \cap (0,1)$ and $0 < \lambda_1 \leq \cdots \leq \lambda_k \to 1$

- Existence for Maxwell-Dirac system $H_D \psi + V_{int}(\psi)\psi = E\psi$

  [Esteban-Georgiev-Sere *Calc.Var. PDE* (1996) , *Abenda* Ann.IHP (1998)]

The variational problem

We look for solutions of the nonlinear eigenvalue problem (P) as the critical points of the *energy functional*

$$\mathcal{E}(\psi) = \|\Lambda_+\psi\|^2_{H^{1/2}} - \|\Lambda_-\psi\|^2_{H^{1/2}} - Ze^2 \int_{\mathbb{R}^3} \frac{\rho_\psi(x)}{|x|}\, dx + \frac{e^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_\psi(x)\rho_\psi(y) - J_\psi(x)\cdot J_\psi(y)}{|x-y|}\, dx\, dy$$

where $\rho_\psi = |\psi|^2$ and $J_\psi = (\psi, \underline{\boldsymbol{\alpha}}\psi)_{\mathbb{C}^4}$, constrained to the set

$$\Sigma = \{\psi \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^4) \,:\, |\psi|^2_{L^2} = 1\}.$$

The (nonlinear) eigenvalue E is the *Lagrange multiplier* :

$$(P) \iff d\mathcal{E}(\psi)[h] = 2E\, \mathrm{Re}\langle\psi|h\rangle_{L^2} \qquad \forall h \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^4)$$

- *Positive eigenvalues*: $E > 0 \iff |\Lambda_-\psi|^2_{L^2} < |\Lambda_+\psi|^2_{L^2}$.

Some useful estimates

- since $|J_\psi(y)| \leq \rho_\psi(y)$ for any $y \in \mathbb{R}^3$, for any $\psi, \phi \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_\psi(y)\rho_\phi(z) - J_\psi(y)\cdot J_\phi(z)}{|y-z|}\, dy\, dz \geq 0.$$

- since $J_\psi \in L^1(\mathbb{R}^3)^3 \cap L^{3/2}(\mathbb{R}^3)^3$ for any $\psi \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{J_\psi(y)\cdot J_\psi(z)}{|y-z|}\, dy\, dz = \frac{1}{\pi}\int_{\mathbb{R}^3} \frac{|\hat{J}_\psi(p)|^2}{|p|^2} \geq 0.$$

- Estimates on commutators:
  Let $\chi \in C_c^\infty(\mathbb{R}^3)$ and $\chi_R(y) = \chi(R^{-1}y)$ then

$$\|[\chi_R, \Lambda_\pm]\|_{H^{1/2}\to H^{1/2}} = O(R^{-1}) \qquad \text{as} \quad R \to +\infty.$$

Idea of the proof

Define the min-max

$$\lambda = \inf_{w\in\Sigma_+} \sup_{\psi\in\Sigma(w)} \mathcal{E}(\psi)$$

where

$$\begin{aligned}\Sigma_+ =& \{w \in X_+ \ : \ |w|^2_{L^2} = 1\}\\ \Sigma(w) =& \{\psi \in \Sigma \ : \ |\psi_+|^{-1}_{L^2}\psi_+ = w\}\\ =& \{\psi = a(\psi_-)w + \psi_-; \ \psi_- \in X_-\},\end{aligned}$$

and $a(\psi_-) = \sqrt{1 - |\psi_-|^2_{L^2}}$, with $\psi_\pm = \Lambda_\pm \psi \in X_\pm$.

To prove that λ is a critical value we show that for any $w \in \Sigma_+$ there exists, unique , $\psi = \psi(w) \in \Sigma(w)$ such that

$$\mathcal{E}(\psi(w)) = \sup_{\psi \in \Sigma(w)} \mathcal{E}(\psi)$$

and that $\mathcal{E}(\psi(w))$ depends smoothly on w.
Then we proceed with the minimization

$$\lambda = \inf_{w \in \Sigma_+} \mathcal{E}(\psi(w)).$$

Remark that the uniqueness is required since the gradient flow is nonlinear and hence deformations do not preserve the linear subspaces structure.

Maximization problem

Proposition.

For any $w \in \Sigma_+$ *there exists, unique,* $\psi = \psi(w) \in \Sigma(w)$*:*

- $\mathcal{E}(\psi(w)) = \sup_{\psi \in \Sigma(w)} \mathcal{E}(\psi) \geq (1 - Ze^2\gamma_T) > 0$;
- *the map* $w \to \mathcal{E}(\psi(w))$ *is smooth;*
- *For any* $h \in span\{w\} \oplus X_-$

$$d\mathcal{E}(\psi(w))[h] - \mu(\psi(w))\, 2\,\mathrm{Re}\langle \psi(w), h\rangle_{L^2} = 0$$

where $\mu(\psi(w)) > 0$ *is the Lagrange multiplier.*

Remark: If ψ is a critical point for $\mathcal{E}$ on $\Sigma(w)$, then

$$\mu(\psi) > 0 \iff |\Lambda_- \psi|^2_{L^2} < \tfrac{1}{2}.$$

Lemma.

Let $B_{1/2} = \{\psi \in \Sigma(w) \ : \ |\Lambda_- \psi|^2_{L^2} < \tfrac{1}{2}\}$ *we have*

- $\mathcal{E}_{|_{\Sigma(w)}}$ *satisfies the Palais Smale condition on* $B_{1/2}$*:*

  $\|\nabla_{\Sigma(w)} \mathcal{E}(\psi_n)\| \to 0$, $\mathcal{E}(\psi_n)$ *bdd* $\Rightarrow$ ψ_n *is precompact in* $B_{1/2}$.

- *If* ψ *is a critical point for* $\mathcal{E}_{|_{\Sigma(w)}}$ *in* $B_{1/2}$

  $$d^2\mathcal{E}(\psi)[h; h] - 2\mu(\psi)|h|^2_{L^2} \leq -\delta \|h\|^2_{H^{1/2}} \qquad \forall h \in T_\psi \Sigma(w)$$

  - *All critical points of* $\mathcal{E}_{|_{\Sigma(w)}}$ *in* $B_{1/2}$ *are strict local maxima.*

Sketch of the proof: Existence

- if $\{\psi_n\}$ is a *maximizing (PS)-sequence* for $\mathcal{E}_{|_{\Sigma(w)}}$ then

$$\psi_n \in B_{1/2}, \text{ definitely.}$$

- $\mathcal{E}_{|_{\Sigma(w)}}$ satisfies the *Palais Smale condition* on $B_{1/2}$:

- By *Ekeland's variational principle* there exists a maximizing (PS)-sequence $\{\psi_n\}$ for $\mathcal{E}_{|_{\Sigma(w)}}$. Then $\{\psi_n\} \subset B_{1/2}$ and hence $\{\psi_n\}$ converge to a maximizer $\psi \in B_{1/2}$.

Sketch of the proof: Uniqueness

Suppose we have two maximizer $\psi_1 \neq \psi_2$, clearly $\psi_1, \psi_2 \in B_{1/2}$. Since

- $B_{1/2}$ is *invariant* for the *gradient flow of* $\mathcal{E}_{|_{\Sigma(w)}}$

then the set

$\Gamma = \{ \gamma \colon [0,1] \to B_{1/2} \mid \gamma(0) = \psi_1,\ \gamma(1) = \psi_2 \} \neq \emptyset$ is *invariant*.

We can then apply the *Mountain Pass theorem* and since the *(PS)-condition* holds in $B_{1/2}$ there exists at the min-max level

$$c = \sup_{\gamma \in \Gamma} \min_{t \in [0,1]} \mathcal{E}(\gamma(t))$$

a critical point of MP-type. We reach a contradiction since

- all critical points of $\mathcal{E}_{|_{\Sigma(w)}}$ in $B_{1/2}$ are *strict local maxima*.

Sketch of the proof: Smoothness

To prove that $w \to \mathcal{E}(\psi(w))$ is *smooth* we use the *Implicit function theorem*. Let $F : \Sigma_+ \times X_- \to H^{-1/2}$

$$F(w, \psi_-) = d\mathcal{E}(\psi)[\,\cdot\,] - \mu(\psi)\, 2\,\mathrm{Re}\langle \psi, \,\cdot\,\rangle_{L^2}$$

with $\psi = a(\psi_-)w + \psi_-$.

- $F(w, \psi_-(w))_{|_{T_\psi \Sigma(w)}} = 0$ if $\psi \in X(w)$ is the maximizer.
- the quadratic form $Q : T_\psi\Sigma(w) \times T_\psi\Sigma(w) \to \mathbb{R}$ given by

$$\begin{aligned} Q(h,k) &= -\langle d_{\psi_-} F(w, \psi_-(w))[h] | k\rangle \\ &= -(d^2\mathcal{E}(\psi(w))[h,k] - \mu(\psi(w))\, 2\,\mathrm{Re}\langle h, k\rangle_{L^2}) \end{aligned}$$

  is *coercive*, hence $d_{\psi_-} F(w, \psi_-(w))$ is invertible.
- by IFT and *uniqueness*, the map $w \to \psi_-(w)$ is *smooth*.

Minimization problem

$$\lambda = \inf_{w\in\Sigma_+} \sup_{\psi\in\Sigma(w)} \mathcal{E}(\psi) = \inf_{w\in\Sigma_+} \mathcal{E}(\psi(w))$$

Proposition.

There exists $w_0 \in \Sigma_+$ *such that* $\psi_0 = \psi(w_0)$ *satisfies*

- $\lambda = \mathcal{E}(\psi_0) = \inf_{w\in\Sigma_+} \mathcal{E}(\psi(w))$
- $E_0 = \mu(\psi_0) \in \mathbb{R}_+ \setminus \sigma(H_D)$ *satisfies*

$$\begin{cases} d\mathcal{E}(\psi_0)[h] = 2E_0 \,\mathrm{Re}\langle\psi_0, h\rangle_{L^2} & \forall h \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^4) \\ |\psi_0|_{L^2} = 1. \end{cases}$$

Sketch of the proof

- By the *Ekeland's variational principle* there exists a *minimizing (PS)- sequence* $\{w_n\} \subset \Sigma_+$:

  Hence $\psi_n = \psi(w_n) \rightharpoonup \psi_0$ (weakly), $\mu(\psi_n) \to \mu_0$ and

  $$d\mathcal{E}(\psi_0)[h] - \mu_0 \, 2 \, \mathrm{Re}\langle \psi_0 \mid h \rangle_{L^2} = 0, \quad \forall h \in H^{1/2}.$$

  - But we do not know if $|\psi_0|_{L^2} = 1$ (not even if $\psi_0 \neq 0$).

Remark.

Since the potential term of the energy functional is weakly continuous, we get *strong convergence* if the (nonlinear) eigenvalue (here the Lagrange multiplier μ_0) is in *the spectral gap* of H_D (exactly as in the linear case $H_D + V_{ext}$).

Lemma.
If $Z > 4$ then $\mu_0 < 1$.

- By the *smooth variational principle of Borwein-Preiss* there exists a *minimizing (PS)- sequence* $\{w_n\} \subset \Sigma_+$ that satisfies

$$d_w^2\mathcal{E}(\psi(w_n))[h_n, h_n] - \mu(\psi_n)2a_n^2|h_n|_{L^2}^2 \geq o_n(1)$$

  for all $h_n \in T_{w_n}\Sigma_+$, with $\psi_n = \psi(w_n)$ and $a_n = |\Lambda_+\psi_n|_{L^2}$.

- for any $\varepsilon > 0$ there exists $h_n^{(\varepsilon)} \in T_{w_n}\Sigma_+$ such that

$$\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\psi_n|^2(x)|h_n^{(\varepsilon)}|^2(y)}{|x-y|} \leq \int_{\mathbb{R}^3} \frac{|h_n^{(\varepsilon)}|^2(y)}{|y|} + o_\varepsilon(\varepsilon) + o_n(1)$$

  and we derive

$$d_w^2\mathcal{E}(\psi_n)[h_n^{(\varepsilon)}, h_n^{(\varepsilon)}] - 2a_n^2|h_n^{(\varepsilon)}|_{L^2}^2 \leq C(4 - Z)\varepsilon + o_\varepsilon(\varepsilon) + o_n(1).$$

- *Work in progress*: The Maxwell-Dirac-Fock equations.

Hartree-Fock : E.H.Lieb, B.Simon CMP (1977); P.L.Lions CMP (1987)

Dirac-Fock : M.J. Esteban, E. Séré CMP (1999)

- *N - relativistic electrons* represented by a *Slater determinant* of ψ_j ($j = 1, \ldots, N$) such that $\langle \psi_j, \psi_k \rangle_{L^2} = \delta_{jk}$.

  Interactions:

  - *nucleus - electron* : $V_{ext}(x) = -\frac{Ze^2}{|x|}$
  - *between electrons* : the electromagnetic potential $A_\mu^{(j)}$ is generated by the static Dirac-current of the N-electrons wave function.

$$\begin{cases} -\Delta A_0^{(j)} = 4\pi e\, \rho_\Psi \\ -\Delta \underline{A}^{(j)} = 4\pi e\, \underline{J}_\Psi \end{cases}$$

where $\rho_\Psi = \sum_{k=1}^N |\psi_k|^2$ and $J_\Psi = \sum_{k=1}^N (\psi_k, \underline{\boldsymbol{\alpha}}\psi_k)_{\mathbb{C}^4}$.

The nonlinear eigenvalue problem

We have a nonlinear, *constrained* system of equations

$$(P)\quad \begin{cases} (H_D + V_{ext})\psi_j + V_{int}(\Psi)\psi_j = \varepsilon_j \psi_j \\ \langle \psi_j, \psi_k \rangle_{L^2} = \delta_{jk} \qquad j,k = 1,\ldots,N \end{cases}$$

where

$$V_{int}(\Psi) = e^2 \rho_\Psi * \frac{1}{|x|}\mathbb{I}_4 - e^2 \underline{\boldsymbol{\alpha}} \cdot J_\Psi * \frac{1}{|x|}$$

By the *U(N)-invariance*, the system (P) is equivalent to

$$\begin{cases} (H_D + V_{ext})\psi_j + V_{int}(\Psi)\psi_j = \sum_{k=1}^N \mu_{jk} \psi_k \\ \langle \psi_j, \psi_k \rangle_{L^2} = \delta_{jk} \qquad j,k = 1,\ldots,N \end{cases}$$

for any $M = \{\mu_{jk}\}_{jk}$, $M = M^*$ with eigenvalues ε_j .

The variational problem

Setting $\Psi^t = (\psi_1, \dots, \psi_N) \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^{4N})$ and
$\mathrm{Gram}_{L^2}\Psi = \{\langle \psi_k, \psi_j \rangle_{L^2}\}_{jk}$ we look for (Ψ, M) solutions of

$$\begin{cases} d\mathcal{E}(\Psi)[h] = \mathrm{Tr}(M\, d(\mathrm{Gram}_{L^2}\Psi)[h]) & \forall h \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^{4N}) \\ \mathrm{Gram}_{L^2}\Psi = \mathbb{I} \end{cases}$$

where $M = \{\mu_{jk}\}$ is the matrix of *Lagrange multipliers* and

$$\mathcal{E}(\Psi) = \|\Psi_+\|^2_{H^{1/2}} - \|\Psi_-\|^2_{H^{1/2}} - Ze^2 \int_{\mathbb{R}^3} \frac{\rho_\Psi(x)}{|x|}\, dx + \frac{e^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_\Psi(x)\rho_\Psi(y) - J_\Psi(x)\cdot J_\Psi(y)}{|x-y|}\, dx\, dy$$

with $\|\Psi_\pm\|^2_{H^{1/2}} = \sum_{k=1}^N \|\Lambda_\pm \psi_k\|^2_{H^{1/2}}$, constrained to the set

$$\triangleright\ \Sigma = \{\Psi \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^{4N}) \,:\, \mathrm{Gram}_{L^2}\Psi = \mathbb{I}\}.$$

Note that $\mathcal{E}(\Psi)$ and Σ are *invariant* by the $U(N)$- action.

- *Positive eigenvalues:*

Lemma.

If Ψ is a critical point for $\mathcal{E}$ on Σ, then

$$M = M(\Psi) > 0 \iff \mathbb{I} - 2\,\mathrm{Gram}_{\mathrm{L}^2}\,\Psi_- > 0$$

.

- $(N = 1)$ $\lambda > 0 \Rightarrow E > 0$ and $E > 0 \iff |\Lambda_- \psi|^2_{L^2} < \frac{1}{2}$.

$$\Rightarrow \lambda = \inf_{\substack{w \in X_+ \\ |w|_{L^2}=1}} \sup_{\psi \in \Sigma(w)} \mathcal{E}(\psi) = \inf_{w \in \Sigma_+} \sup_{\psi \in B_{1/2}} \mathcal{E}(\psi)$$

where

$$\Sigma_+ = \{w \in X_+ \;:\; |w|^2_{L^2} = 1\}$$
$$\Sigma(w) = \{\psi \in \Sigma \;:\; |\psi_+|^{-1}_{L^2}\psi_+ = w\}$$
$$B_{1/2} = \{\psi \in \Sigma(w) \;:\; |\Lambda_- \psi|^2_{L^2} < \frac{1}{2}\}$$

- *Min-max:*

For any $N \in \mathbb{N}$, we define

$$\lambda_N = \inf_{w \in \Sigma_+} \sup_{\Psi \in B_{1/2}} \mathcal{E}(\Psi)$$

where

$$\Sigma_+ = \left\{ w \in X_+^N \;\middle|\; \mathrm{Gram}_{L^2} w = \mathbb{I} \right\}$$
$$\Sigma(w) = \left\{ \Psi \in \Sigma \;\middle|\; (\mathrm{Gram}_{L^2} \Psi_+)^{-1/2} \Psi_+ = Uw;\; U \in U(N) \right\}$$
$$B_{1/2} = \{ \Psi \in \Sigma(w) \;:\; \mathbb{I} - 2\mathrm{Gram}_{L^2} \Psi_- > 0 \}$$

Note that $\Sigma_+, \Sigma(w), B_{1/2}$ are *invariant* by the $U(N)$- action.

- $\mathcal{E}_{|_{\Sigma(w)}}$ satisfies the *Palais Smale condition* on $B_{1/2}$.

Proposition. (*Maximization problem*)

For any $w \in \Sigma_+$ there exists $\Psi(w) \in B_{1/2}$:

- $\mathcal{E}(\Psi(w)) = \sup_{\psi \in B_{1/2}} \mathcal{E}(\Psi) \geq (1 - Z\alpha_{fs}\gamma_T) > 0$;
- *For any $h \in (W \oplus X_-)^N$, where $W = span\{w_1, \cdots, w_n\}$*

$$d\mathcal{E}(\Psi(w))[h] - Tr(M(\Psi(w))d(Gram_{L^2}\Psi)[h]) = 0$$

  and the Lagrange multipliers matrix $M(\Psi(w))$ is positive definite.

- In progress: If Ψ is a *critical point* for $\mathcal{E}|_{\Sigma(w)}$ in $B_{1/2}$ then

$$d^2\mathcal{E}(\Psi)[h; h] - 2\mathrm{Tr}(M(\Psi)\mathrm{Gram}_{L^2} h) \leq -\delta \|h\|^2_{H^{1/2}}$$

  for any $h \in T_\Psi \Sigma(w)$.
- *Open question*: *Uniqueness* for the maximizer $\Psi(w)$ and the *smoothness* of $w \to \mathcal{E}(\psi(w))$.

Proposition. (*Minimization problem*)

- *Suppose that the map* $w \to \mathcal{E}(\psi(w))$ *is smooth then*

$$\lambda = \inf_{w\in\Sigma_+} \sup_{\psi\in\Sigma(w)} \mathcal{E}(\psi) = \inf_{w\in\Sigma_+} \mathcal{E}(\psi(w))$$

There exists $w_0 \in \Sigma_+$ *such that* $\Psi_0 = \Psi(w_0)$ *satisfies*

- $\lambda = \mathcal{E}(\Psi_0) = \inf_{w\in\Sigma_+} \mathcal{E}(\psi(w))$
- $M(\Psi_0) > 0$ *and* $\mathbb{I} - M(\Psi_0) > 0$,

$$\Rightarrow \varepsilon_j \in \mathbb{R}_+ \setminus \sigma(H_D);$$

and

$$\begin{cases} d\mathcal{E}(\Psi_0)[h] = Tr(M(\Psi_0) d\, Gram_{L^2}\Psi_0[h]) \\ Gram_{L^2}\Psi_0 = \mathbb{I}. \end{cases}$$

for any $h \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^{4N})$.

Thanks for the attention!