On the MIT bag model :
Self-adjointness and non-relativistic limits

Loïc Le Treust

Maître de conférences at Aix-Marseille university.

Joint work with :

Naiara Arrizabalaga, Universidad del País Vasco.
Nicolas Raymond, Université de Rennes 1.

Roma, September 2017

Introduction

Non-relativistic particles confined in a box

$$\inf\{\lambda_d^1(\Omega) + b|\Omega|, \quad \Omega \text{ open subset of } \mathbb{R}^3\},$$

- $\lambda_d^1(\Omega)$: Kinetic energy given by the 1^{st} eig. of the Dirichlet Laplacian,
- $|\Omega|$: energy of the box given by its volume,
- $b > 0$: coupling constant.

Rk : The solution is a ball (unique up to translation).
Rk : Toy model in quantum physics ?
$\rightsquigarrow$ Quarks are perfectly confined (ex : protons, neutrons).

Non-relativistic approximation not valid for (light) quarks

$$-\Delta \text{ (Schrödinger's Op.)} \rightsquigarrow H \text{ (Dirac's Op.)}$$

Physical context :

Confinement of quarks, anti-quarks, gluons inside the hadrons.

- The quarks and anti-quarks are fermions (elementary particles ?),
- The elementary force involved : the strong force,
- The gluons are the associated gauge bosons,
- The hadrons are composite particles. Ex : neutrons, protons, mesons (gauge bosons for the strong nuclear force),...

Problems

1. Define the operator related to the kinetic energy of confined relativistic particles $\rightsquigarrow$ MIT bag Dirac operator.
2. Study the self-adjointness and its properties (asymptotic analysis).
3. ...
4. Study the associated shape optimization problem.
5. Study the uniqueness of the shape (up to symmetries).

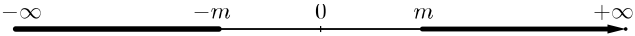
Dirac's operator on $\mathbb{R}^3$

- $H = -i\sum_{k=1}^{3}\alpha_k\partial_k + \beta m = -i\alpha.\nabla + \beta m$, $\begin{cases} m \in \mathbb{R}, \text{ (mass)}, \\ (\alpha_1, \alpha_2, \alpha_3), \beta \in \mathbb{C}^{4\times 4} \text{ hermit.} \end{cases}$

self-adj. on $L^2(\mathbb{R}^3, \mathbb{C})^4$,

$$H^2 = -\Delta + m^2$$

$\sigma(\mathrm{H}_0)$



$\rightsquigarrow$ Problems with negative spectrum ?

- $[m, +\infty)$ is related to kinetic energy of particles,
- $(-\infty, -m]$ is related to kinetic energy of antiparticles.

Notation

$$\alpha \cdot A = \sum_{k=1}^{3}\alpha_k A_k$$

for $A = (A_1, A_2, A_3)$.

[Tha91] Thaller. *The Dirac equation.* (1991). Texts and Monographs in Physics.

MIT bag Dirac operator on Ω

$(H_m^\Omega, \mathrm{Dom}(H_m^\Omega))$ is defined on the domain

$$\mathrm{Dom}(H_m^\Omega) = \{\psi \in H^1(\Omega, \mathbb{C}^4) \ : \ \mathcal{B}\psi = \psi \text{ on } \partial\Omega\},$$

by $H_m^\Omega \psi = H\psi$ for all $\psi \in \mathrm{Dom}(H_m^\Omega)$ where

$$\mathcal{B}(x) = -i\beta\alpha \cdot \mathbf{n}(x), \quad \forall x \in \partial\Omega\},$$

n is the outward pointing normal to $\partial\Omega$ (regular).

Physical interpretation of the boundary cond. :

$\rightsquigarrow$ no normal quantum current at the boundary.

[CJJ+74] Chodos, Jaffe, Johnson, Thorn, Weisskopf. *New extended model of hadrons* (1974). Phys. Rev. D.
[Joh75] Johnson. *The MIT bag model.* (1975) Acta Phys. Pol.

Remarks on the boundary condition

1. One of the simplest local boundary condition for H_m^Ω to be symmetric,
   $\rightsquigarrow$ Despite its simplicity, it has been very successful for calculating some physical quantities.

2. The trace is well-defined by a classical trace theorem.

3. The spectrum of the matrix $\mathcal{B}$ is ± 1 : $\mathcal{B}^* = \mathcal{B}$ and $\mathcal{B}^2 = 1_4$,
   $\rightsquigarrow$ Another choice for the boundary condition is $\mathcal{B}\psi = -\psi$: no normal quantum current, equivalent to considering inward pointing normal, the associated Dirac op. is symmetric.

4. Spontaneous chiral symmetry breaking.
   $\rightsquigarrow$ The chirality matrix $\gamma_5 = -i\alpha_1\alpha_2\alpha_3$ satisfies

$$\gamma_5^2 = 1_4,\ \gamma_5(-i\alpha\cdot\nabla + m\beta)\gamma_5 = -i\alpha\cdot\nabla - m\beta \text{ and } \gamma_5\mathcal{B}\gamma_5 = -\mathcal{B}.$$

Theorem

i. $(H, \mathrm{Dom}(H))$ *is a self-adjoint operator with compact resolvent.*

ii. *We denote by* $(\mu_n(m))_{n\geq 1} \subset \mathbb{R}_+^*$ *the eigenvalues of* $|H|$. *The spectrum of* H, *denoted by* $\mathrm{sp}(H)$, *is symmetric with respect to* 0 *(with multiplicity) and*

$$\mathrm{sp}(H) = \{\pm\mu_n(m),\ n \geq 1\}.$$

iii. *Each eigenvalue of* H *has even multiplicity.*

iv. *For each* $\psi \in \mathrm{Dom}(H)$, *we have*

$$\|H\psi\|^2_{L^2(\Omega)} = \|\alpha\cdot\nabla\psi\|^2_{L^2(\Omega)} + m\|\psi\|^2_{L^2(\partial\Omega)} + m^2\|\psi\|^2_{L^2(\Omega)},$$

and

$$\|\alpha\cdot\nabla\psi\|^2_{L^2(\Omega)} = \|\nabla\psi\|^2_{L^2(\Omega)} + \frac{1}{2}\int_{\partial\Omega}\kappa|\psi|^2 dx.$$

where κ *is the sum of the principal curvatures.*

For the 2D case but $\neq$ proof : Spectral gaps of Dirac operators with boundary conditions relevant for graphene. **Benguria, Fournais, Stockmeyer, Van Den Bosch** .(2016).

Some steps in the proofs.

1. Symmetries and multiplicity
   $\rightsquigarrow$ come from the properties of the matrices $\alpha_1, \alpha_2, \alpha_3$ and β.

2. The formulas for the quadratic form of H^2.
   $\rightsquigarrow$ come from integrations by parts and

$$[\alpha \cdot (\mathbf{n} \times D), \mathcal{B}] = -\kappa\gamma_5\mathcal{B}$$

   where $D = -i\nabla$.

3. The self-adjointness and in particular the proof of $\mathcal{D}(H^*) \subset H^1(\Omega)$.
   $\rightsquigarrow$ comes from the existence of an extension operator

$$\mathcal{D}(H^*) \longrightarrow H^1(\mathbb{R}^3) \longrightarrow H^1(\Omega).$$

4. The compact resolvent property
   $\rightsquigarrow$ comes form the compact Sobolev embeddings.

The limit m tends to $+\infty$.

Theorem (N. Arrizabalaga, L.L.T., N. Raymond)

Let $-\Delta^{\mathrm{Dir}}$ be the Dirichlet Laplacian with domain $H^2(\Omega,\mathbb{C}^4)\cap H^1_0(\Omega,\mathbb{C}^4)$, and let $(\mu_n^{\mathrm{Dir}})_{n\geq 1}$ be the non-decreasing sequence of its eigenvalues. For all $n\geq 1$, we have

$$\mu_n(m)-\left(m+\frac{1}{2m}\mu_n^{\mathrm{Dir}}\right)\underset{m\to+\infty}{=}o\left(\frac{1}{m}\right).$$

Element of proof : Pre-compactness of the sequences of eigenfunctions.

Theorem (N. Arrizabalaga, L.L.T., N. Raymond)

Let $u_1\in H^1_0(\Omega,\mathbb{C})$ be a L^2-normalized eigenfunction of the Dirichlet Laplacian associated with its lowest eigenvalue μ_1^{Dir}. We have

$$\mu_1(m)-\left(m+\frac{1}{2m}\mu_1^{\mathrm{Dir}}-\frac{1}{2m^2}\int_{\partial\Omega}|\partial_{\mathbf{n}}u_1|^2dx\right)\underset{m\to+\infty}{=}o\left(\frac{1}{m^2}\right).$$

Element of proof :

- [Upper bound] formal asymptotic expansion and Fredholm alternative.

The limit m tends to $-\infty$.

1. The boundary is attractive for the eigenfunctions with eigenvalues lying essentially in the Dirac gap $[-|m|, |m|]$.

2. The distribution of the eigenfunctions is governed by the boundary operator

$$\mathcal{L} - \frac{\kappa^2}{4} + K$$

where κ and K are the trace and the determinant of the Weingarten map, respectively, and where $\mathcal{L}$ is defined as follows.

Definition

The operator $(\mathcal{L}, \mathrm{Dom}(\mathcal{L}))$ is the self-adjoint operator associated with the quadratic form

$$\mathcal{Q}(\psi) = \int_{\partial\Omega} \|\nabla_s \psi\|^2 dx\,, \quad \forall \psi \in H^1(\partial\Omega, \mathbb{C})^4 \cap \ker(\mathcal{B} - 1_4)\,.$$

Theorem (N. Arrizabalaga, L.L.T., N. Raymond)

Let $\varepsilon_0 \in (0,1)$ *and*

$$\mathsf{N}_{\varepsilon_0, m} := \{n \in \mathbb{N}^* : \mu_n(-|m|) \leq |m|\sqrt{1-\varepsilon_0}\}\,.$$

There exist C_-, C_+, m_0 *such that, for all* $|m| \geq m_0$ *and* $n \in \mathsf{N}_{\varepsilon_0, m}$,

$$\mu_n^-(|m|) \leq \mu_n(-|m|) \leq \mu_n^+(|m|)\,,$$

with $\mu_n^\pm(|m|)$ *being the non-decreasing sequence of eigenvalues of the operators* $L_m^\pm$ *of* $L^2(\partial\Omega, \mathbb{C})^4$ *defined by*

$$L_m^- = \left([1 - C_-|m|^{-\frac{1}{2}}]\mathcal{L} - \frac{\kappa^2}{4} + K - C_-|m|^{-1}\right)_+^{\frac{1}{2}}\,,$$

$$L_m^+ = \left([1 + C_+|m|^{-\frac{1}{2}}]\mathcal{L} - \frac{\kappa^2}{4} + K + C_+|m|^{-1}\right)^{\frac{1}{2}}\,.$$

Corollary

For all $n \in \mathbb{N}^*$, we have that

$$\mu_n(-|m|) \underset{m\to+\infty}{=} \widetilde{\mu}_n^{\frac{1}{2}} + \mathcal{O}(|m|^{-\frac{1}{2}}),$$

where $(\widetilde{\mu}_n)_{n\in\mathbb{N}^*}$ is the non-decreasing sequence of the eigenvalues of the following non-negative operator on $L^2(\partial\Omega,\mathbb{C})^4 \cap \ker(1_4 - \mathcal{B})$:

$$\mathcal{L} - \frac{\kappa^2}{4} + K.$$

An inspiration : Weyl formulae for the Robin Laplacian in the semiclassical limit
A. Kachmar, **P. Keraval** and **N. Raymond**. Confluentes Mathematici (2017).

Other works for the Robin Laplacian by : **Exner**, **Freitas**, **Helffer**, **Kachmar**, **Krejčiřík**, **Levitin**, **Minakov**, **Pankrashkin**, **Parnovski**, **Popoff**,...

Ingredients of the proof

1. Agmon estimates : exponential confinement at the boundary.

   $\rightsquigarrow$ using tests functions of the form

$$\psi_m^n(\cdot)\exp\left(-|m|\gamma \mathrm{d}(\cdot,\partial\Omega)\right)$$

   where

   - ψ_m^n is an eigenfunction whose eigenvalue $\mu_n(-|m|)$ satisfies
   $$\mu_n(-|m|) \leq |m|\sqrt{1-\varepsilon_0}\,,$$
   - $\gamma \in (0, \sqrt{\varepsilon_0})$ and $\varepsilon_0 \in (0,1)$,
   - d is the euclidean distance.

2. Tubular coordinates near the boundary and semiclassical rescaling.

   $\rightsquigarrow$ using the parameters $(s,\tau) \in \partial\Omega \times \mathbb{R}_+$ where

$$x = s - |m|^{-1}\tau\mathbf{n}(s)$$

   for $x \in \Omega$ s.t. $\mathrm{d}(x, \partial\Omega)$ is small enough.

3. Born-Oppenheimer reduction : multiscales analysis.
   - the leading order op. forces the confinement near the boundary (acts in the normal direction).
   - the next scale contributions give us the operator acting on the s-variable.

Grazie ! Thanks !

Arrizabalaga, N. ; Le Treust, L. ; Raymond, N. **On the MIT bag model in the non-relativistic limit**. Comm. Math. Phys. 354 (2017), no. 2, 641–669.