Non linear models from relativistic quantum mechanics : spectral and asymptotic analysis and related problems.

Nabile Boussaid

Modèles non linéaires issus de la mécanique quantique relativiste : analyse spectrale, asymptotique et problèmes associés.

Projet d'habilitation à diriger des recherches
Mathématiques appliquées et applications des mathématiques

---

présenté par Nabile Boussaïd

Jury

Rapporteurs: **Jean-Michel Coron**
Professeur, Université Pierre et Marie Curie

Marco Marletta
Professor, University of Cardiff

Nikolay Tzvetkov
Professeur, Université de Cergy-Pontoise

Examinateurs: **Anne de Bouard**
Directrice de Recherche, École Polytechnique

Mariana Hărăguş
Professeur, Université de Franche-Comté

Florian Méhats
Professeur, Université de Rennes 1

Éric Séré
Professeur, Université Paris-Dauphine

Université de Franche-Comté, U.F.R Sciences et Techniques

Contents

Part I

Introduction

I.1

Introduction

Dans ce mémoire, je présenterai les différents travaux de recherche que j'ai menés depuis la soutenance de mon doctorat [Bou06a]. Dans cette dernière, j'analysais la stabilité de solutions stationnaires d'une classe d'équations de Dirac non-linéaires [Bou06b ; Bou08 ; Bou07]. Les aspects relativistes de ces équations ne permettant pas de donner un sens clair à la notion d'état fondamental, l'analyse de la stabilité au sens de Lyapounov des solutions stationnaires était compromise.

Nous avions contourné cette difficulté en considérant la notion plus forte de stabilité dynamique ou asymptotique. Au préalable, il fallait montrer la stabilité spectrale en utilisant des méthodes de bifurcations à partir de problèmes linéaires *ad hoc*. Nous nous étions donc restreints aux petites solutions stationnaires.

Un partie importante de l'analyse menée durant cette thèse relevait de la théorie spectrale. Cela est évident dans l'étude de la stabilité spectrale. En effet, la problématique est l'analyse des valeurs propres isolées et de multiplicités finies de l'opérateur linéarisé. De manière moins évidente, l'obtention de la dynamique de l'équation linéarisée sur le reste du spectre utilise des outils sophistiqués de l'analyse du spectre essentiel. Les propriétés de l'opérateur résolvante par des méthodes de Mourre, ou de développement en valeurs propres généralisées, furent ainsi des outils essentiels.

Dès lors que la théorie linéaire ou linéarisée fut comprise, il nous restait à établir les propriétés dynamiques de nos solutions en considérant des formulations de Cauchy bien choisies dans le cadre fonctionnel donné par l'analyse linéaire.

À partir de ma thèse, j'ai envisagé différentes directions de recherche en accord avec le contexte scientifique dans lequel j'évoluais.

Lors de mon séjour postdoctorat à l'Université Heriot-Watt (Edimbourg) sous l'influence de Lyonell Boulton et Michael Levitin, j'ai considéré des questions liées à l'analyse numérique d'opérateurs autoadjoints dont le spectre n'est borné ni inférieurement, ni supérieurement ou plus généralement d'opérateurs autoadjoints avec du spectre discret dans les trous du spectre essentiel. Le but était de mettre en œuvre une caractérisation du spectre discret menant à une implémentation numérique.

La pollution spectrale est un phénomène numérique théorique. Il relève de l'analyse numérique puisqu'il apparaît lorsque l'on tente d'approcher le spectre discret d'un opérateur (en dimension infinie) par celui d'une suite de matrices (en général ses compressions à une suite d'espaces dont les dimensions vont croissantes). Il est seulement théorique puisque il apparaît dans l'adhérence d'une suite de spectres discrets. La pollution spectrale est la partie de cette adhérence qui n'est pas dans le spectre.

Tant qu'une valeur propre peut être caractérisée par un principe de min-max classique, elle peut toujours être approchée raisonnablement par le spectre des compressions. Concrètement, seul le bas du spectre discret possède une telle caractérisation. Si, comme dans le cas de l'opérateur de Dirac, le spectre n'est pas borné inférieurement ou supérieurement une telle caractérisation n'est pas simple ou pas simple d'usage. C'est donc assez naturellement que Lyonell Boulton et moi-même avions envisagé une autre caractérisation du spectre donnant également une méthode numérique. Nous avons donc analysé l'implémentation numérique de la méthode du second ordre avec une base de Hermite pour approcher le spectre discret d'opérateurs de Dirac [BB10]. L'intérêt essentiel de notre analyse est de proposer une méthode permettant d'obtenir un encadrement des éléments du spectre discret. Cet encadrement intersecte nécessairement le spectre et est de ce fait exempt de toute pollution spectrale.

Notons que la méthode d'approximation par les spectres des compressions, dite méthode de Galerkin, basée sur la caractérisation de Rayleigh-Ritz, ou min-max, est toujours utilisable dans le cas de l'opérateur de Dirac tout en étant possiblement sujette à la pollution. La pollution spectrale dépend de la suite de sous-espaces considérée pour les compressions. Pour un nombre de cas important, soit il n'y a pas de pollution spectrale soit cette pollution est bien localisée et disjointe du spectre discret (cf. Lewin & Séré [LS10]). Toujours en référence à [LS10], il est possible de caractériser les suites de sous-espaces exempts de pollution spectrale. De tels critères sont assez connus par la communauté des chimistes. Il semble que la méthode de Galerkin construite sur une base de Hermite ne présente pas de pollution spectrale bien que nous n'ayons aucun critère pour le prouver. Nos réflexions dans cette direction nous ont menés à une collaboration avec Lyonell Boulton et Mathieu Lewin sur les propriétés de la pollution spectrale [BBL12]. La question qui nous intéressait était la stabilité de cette dernière par perturbation relativement compact. Nous avons alors obtenu un théorème de stabilité de type Weyl.

Nous avions à l'époque financé cette collaboration par un accord de partenariat Hubert Curien. Ceci a permis de financer un autre projet, celui mené avec Gabriel Barrenechea et Lyonell Boulton sur le calcul numérique des modes propres des équations de Maxwell dans une cavité résonnante [BBBa ; BBBb]. Les opérateurs associés aux équations de Maxwell ont également un spectre qui n'est borné ni inférieurement ni supérieurement. Ils présentent aussi la particularité d'avoir un noyau infiniment dégénéré si la loi de Gauß n'est pas incluse. D'un point de vue numérique ceci représente un ensemble de difficultés bien connues. Nous avons envisagé la question avec la contrainte d'imposer un minimum de conditions sur le modèle et sur la méthode. Nous avons étudié et amélioré une méthode due à Zimmermann et Mertins.

Dans le cadre des questions liées aux propriétés dynamiques des opérateurs linéarisés, j'utilisais de manière essentielle le principe d'absorption limite, une estimation de l'opérateur résolvante au voisinage du spectre dans des espaces pondérés. C'est une question similaire qui nous a intéressés, avec Sylvain Golénia pour des perturbations de type longue portée. Nous avons démontré dans cette analyse un principe d'absorption limite au voisinage des seuils [BG10]. Nous avions alors utilisé une méthode de Mourre faible afin de traiter les énergies aux seuils et gagner la positivité en utilisant le complément de Schur qui fait apparaître, d'une certaine manière, la limite non relativiste.

Peu de temps après, j'ai eu l'occasion de découvrir une autre méthode liée à des commutateurs. C'est la méthode des multiplicateurs de Morawetz. Ce fut à l'occasion de ma rencontre avec Piero d'Anconna et Luca Fanelli qui avaient étudié les propriétés dispersives de perturbations de l'opérateur de Dirac. Nous avions alors étudié des perturbations magnétiques et obtenu des estimations de Morawetz et de Strichartz [BDF11].

Dans la lignée de mes travaux sur la stabilité spectrale, j'ai, à l'occasion de ma rencontre avec Scipio Cuccagna, commencé une collaboration sur l'extension de mes travaux de doctorat au cas dit résonnant [BC12b]. Il faut noter que dans le cadre de mes études doctorales, je m'étais limité à une analyse linéaire et les aspects non linéaires étaient vus de manière perturbative. Or depuis les travaux fondateurs (en ce qui concerne le cas des équations dispersives) de Soffer & Weinstein, on sait que des phénomènes de résonances non linéaires peuvent stabiliser ou déstabiliser certains équilibres dans des équations d'évolutions dispersives. De tels phénomènes, dans le cas des équations des ondes, de Klein-Gordon ou même de Schrödinger, sont en fait dus à un couplage non linéaire entre des modes discrets et le spectre essentiel du linéarisé autour d'un équilibre. Dans le cas de l'équation de Schrödinger, le caractère réversible de l'équation donne un spectre essentiel qui est en fait la réunion de deux copies de signes opposés de $[|\omega|, \infty)$ (si on considère un état stationnaire de niveau ω comme équilibre). Dans le cas de l'équation de Dirac ce sont donc des copies de translations de $\mathbb{R} \setminus (-m; m)$ que l'on obtient. Le spectre de la linéarisation est donc divisé en trois parties, un partie libre de spectre essentiel, une partie doublement couverte par le spectre essentiel (qui est non bornée) et entre les deux une partie simplement couverte. Lorsque le premier ordre de couplage entre les modes discrets et le spectre essentiel se fait au niveau de la partie simplement couverte, une analyse similaire à celle de l'équation de Schrödinger nous permet de montrer que les phénomènes de résonance non-linéaire tendent à stabiliser le système.

Néanmoins, l'analyse que nous avions menée avec Scipio Cuccagna s'est faite au prix d'hypothèses importantes sur le spectre de l'opérateur linéarisé. C'est un choix qui s'inscrivait dans une logique à plus long terme. Il s'agissait de comprendre ce qui était possible de faire au niveau non linéaire et avec quels jeux d'hypothèses acceptables. Depuis j'étudie la faisabilité de ces hypothèses. Il reste toujours beaucoup de questions ouvertes mais la question du spectre de l'opérateur linéarisé a fait l'objet d'une collaboration avec Andrew Comech qui nous a permis de clarifier partiellement la situation [BC12a]. Une des difficultés rencontrées est encore liée au caractère non coercitif de l'opérateur de Dirac. Le spectre ne peut plus être confiné aux axes réel et imaginaire comme dans le cas de l'équation de Schrödinger non linéaire. Les mécanismes qui peuvent donner de l'instabilité sont donc plus complexes.

En dernier lieu et avant de clore cette introduction, il me faut mentionner mes travaux liés à des problématiques de contrôle bilinéaire en mécanique quantique [BCC13c ; BCC14c ; BCC14a ; BCC12a ; BCC12b ; BCC12c ; BCC12e ; BCC12d ; BCC12a ; BCC13a ; BCC13b ; BCC14b]. Cet ensemble fut mené en collaboration avec Marco Caponigro et Thomas Chambrion. La question de départ fut posée par Thomas Chambrion lors d'un de ses exposés à l'université de Franche-Comté. La question qui semblait les intéresser était celle de la construction de solutions de problèmes d'évolutions linaires non autonomes avec une régularité temporelle faible. Cette question et un certain nombre de problèmes connexes nécessitent une analyse assez fine des propriétés d'opérateurs non bornés. Nous avons étendu à un cadre plus général un certain nombre de résultats désormais classiques.

> In re mathematica ars proponendi quaestionem pluris facienda est quam solvendi.
>
> Titre de la troisième soutenance de la thèse de Georg Cantor *De aequationibus secundi gradus indeterminatis* [Dissertation, Friedrich-Wilhelms-Universität, Berlin, 1867].

Remerciements

Je voudrais dans ce court paragraphe remercier Jean-Michel Coron, Nikolay Tzvetkov et Marco Marletta pour avoir rapporté ce manuscrit, pour leurs lectures attentives et le temps qu'il y ont consacré. Je suis tout autant reconnaissant à Anne de Bouard, Mariana Haragus, Florian Méhats et Éric Séré d'avoir accepté d'être examinateurs.

Ce travail n'aurait pas été possible sans la patience de mes collaborateurs et les nombreuses heures de travail en commun. Je remercie donc (par ordre alphabétique) : Gabriel, Lyonell, Marco, Thomas, Andrew, Scipio, Piero, Luca, Sylvain et Mathieu. Je n'oublie pas ceux dont les travaux en cours n'ont pas pu être inclus ici.

L'environnement enrichissant du laboratoire de mathématiques de Besançon fut aussi un élément essentiel à l'aboutissement de ce travail. Je remercie tous mes collègues et en particulier ceux de l'équipe EDP.

Merci à Sohayl, Abaan et Sopheak.

Références

[LS10] M. Lewin et É. Séré. « Spectral pollution and how to avoid it (with applications to Dirac and periodic Schrödinger operators) » . In : *Proc. Lond. Math. Soc. (3)* 100.3 (2010), p. 864–900. DOI : 10.1112/plms/pdp046. URL : http://dx.doi.org/10.1112/plms/pdp046.

Thèse

[Bou06a] N. Boussaïd. "Étude de la stabilité des petites solutions stationnaires pour une classe déquations de Dirac non linéaires". Juil. 2006. URL : http://tel.archives-ouvertes.fr/tel-00108459/PDF/These.pdf.

Publications

[Bou06b] N. Boussaïd. « Stable directions for small nonlinear Dirac standing waves » . In : *Comm. Math. Phys.* 268.3 (2006), p. 757–817. DOI : 10.1007/s00220-006-0112-3. URL : http://hal.archives-ouvertes.fr/hal-00016041/PDF/Article-StabilizationSmallDirac%20SolitonNonResonantCaseFinal.pdf.

[Bou08] N. Boussaïd. « On the asymptotic stability of small nonlinear Dirac standing waves in a resonant case » . In : *SIAM J. Math. Anal.* 40.4 (2008), p. 1621–1670. DOI : 10.1137/070684641. URL : http://hal.archives-ouvertes.fr/hal-00116269/PDF/Article-2-StabilizationSmallDir%20acSolitonResonantCaseFinal41.pdf.

[BB10] L. Boulton et N. Boussaïd. « Non-variational computation of the eigenstates of Dirac operators with radially symmetric potentials » . In : *LMS J. Comput. Math.* 13 (2010), p. 10–32. DOI : 10.1112/S1461157008000429. URL : http://hal.archives-ouvertes.fr/hal-00308843/PDF/Preprint-DiracNumerical.pdf.

[BG10] N. Boussaïd et S. Golénia. « Limiting absorption principle for some long range perturbations of Dirac systems at threshold energies » . In : *Comm. Math. Phys.* 299.3 (2010), p. 677–708. DOI : 10.1007/s00220-010-1099-3. URL : http://hal.archives-ouvertes.fr/hal-00392422/PDF/LAPDLRvHAL20090608.pdf.

[BDF11] N. Boussaïd, P. D'Ancona et L. Fanelli. « Virial identity and weak dispersion for the magnetic Dirac equation » . In : *J. Math. Pures Appl. (9)* 95.2 (2011), p. 137–150. DOI : 10.1016/j.matpur.2010.10.004. URL : http://hal.archives-ouvertes.fr/hal-00430346/PDF/diracsmoo-20091218.pdf.

[BBL12] L. Boulton, N. Boussaïd et M. Lewin. “ Generalised Weyl theorems and spectral pollution in the Galerkin method ” . In : *J. Spectr. Theory* 2.4 (2012), p. 329–354. doi : 10.4171/JST/32. url : http://hal.archives-ouvertes.fr/hal-00536270/PDF/Weyl32.pdf.

[BC12b] N. Boussaïd et S. Cuccagna. “ On stability of standing waves of nonlinear Dirac equations ” . In : *Comm. Partial Differential Equations* 37.6 (2012), p. 1001–1056. doi : 10.1080/03605302.2012.665973. url : http://hal.archives-ouvertes.fr/hal-00578790/PDF/StabDirac20120103.pdf.

[BCC13c] N. Boussaïd, M. Caponigro et T. Chambrion. “ Weakly coupled systems in quantum control ” . In : *IEEE Trans. Automat. Control* 58.9 (2013), p. 2205–2216. doi : 10.1109/TAC.2013.2255948.

Prépublications

[Bou07] N. Boussaïd. *A stability result for small stationary solutions of a class of nonlinear Dirac equations*. 2007. url : http://basepub.dauphine.fr/xmlui/handle/123456789/6543.

[BC12a] N. Boussaïd et A. Comech. *On spectral stability of the nonlinear Dirac equation*. 2012. arXiv : 1211.3336 [math.AP].

[BCC14a] N. Boussaïd, M. Caponigro et T. Chambrion. *Approximate controllability of the Schrödinger Equation with a polarizability term in higher Sobolev norms*. Juin 2014. url : http://hal.archives-ouvertes.fr/hal-01006178.

[BCC14b] N. Boussaïd, M. Caponigro et T. Chambrion. *Efficient finite dimensional approximations for the bilinear Schrodinger equation with bounded variation controls*. 2014. url : http://hal.archives-ouvertes.fr/hal-01003056.

[BCC14c] N. Boussaïd, M. Caponigro et T. Chambrion. *Regular propagators of bilinear quantum systems*. Juin 2014. url : http://hal.archives-ouvertes.fr/hal-01016299.

[BBBa] G. R. Barrenechea, L. Boulton et N. Boussaïd. *Eigenvalue enclosures*. url : http://hal.archives-ouvertes.fr/hal-00837475.

[BBBb] G. R. Barrenechea, L. Boulton et N. Boussaïd. *Finite element eigenvalue enclosures for the Maxwell operator*. url : http://hal.archives-ouvertes.fr/hal-00949589.

Actes de conférences avec comité de lecture

[BCC12a] N. Boussaïd, M. Caponigro et T. Chambrion. “ Approximate controllability of the Schrödinger equation with a polarizability term ” . In : *Decision and Control (CDC), 2012 IEEE 51st Annual Conference on*. IEEE. 2012, p. 3024–3029. doi : 10.1109/CDC.2012.6426619. url : http://hal.archives-ouvertes.fr/hal-00784881/PDF/Quadratique13.pdf.

[BCC12b] N. Boussaïd, M. Caponigro et T. Chambrion. “ Implementation of logical gates on infinite dimensional quantum oscillators ”. In : *American Control Conference (ACC), 2012*. IEEE. 2012, p. 5825–5830. url : http://hal.archives-ouvertes.fr/hal-00637115/PDF/QG%5C_ACC%5C_0.6.pdf.

[BCC12c] N. Boussaïd, M. Caponigro et T. Chambrion. “ Periodic control laws for bilinear quantum systems with discrete spectrum ”. In : *American Control Conference (ACC), 2012*. IEEE. 2012, p. 5819–5824. url : http://hal.archives-ouvertes.fr/hal-00637116/PDF/FEPS%5C_ACC%5C_3.pdf.

[BCC12d] N. Boussaïd, M. Caponigro et T. Chambrion. “ Small time reachable set of bilinear quantum systems ” . In : *Decision and Control (CDC), 2012 IEEE 51st Annual Conference on*. IEEE. 2012, p. 1083–1087. doi : 10.1109/CDC.2012.6426208. url : http://hal.archives-ouvertes.fr/hal-00710040/PDF/Time06.pdf.

[BCC12e] N. Boussaïd, M. Caponigro et T. Chambrion. “ Which notion of energy for bilinear quantum systems? ” In : *proceeding of the 4th IFAC Workshop on Lagrangian and Hamiltonian Methods for Non Linear Control, pp 226-230, 29-31 août 2012*. 2012, p. 226–230. doi : 10.3182/20120829-3-IT-4022.00034. url : http://hal.archives-ouvertes.fr/hal-00784890/PDF/Energy4.pdf.

[BCC13a] N. Boussaïd, M. Caponigro et T. Chambrion. “ Energy Estimates for Low Regularity Bilinear Schrödinger Equations ” . In : *Control of Systems Governed by Partial Differential Equations*. T. 1. 1. 2013, p. 25–30. doi : 10.3182/20130925-3-FR-4043.00046. url : http://hal.archives-ouvertes.fr/hal-00784876/PDF/cpde09.pdf.

[BCC13b] N. Boussaïd, M. Caponigro et T. Chambrion. “ Total variation of the control and energy of bilinear quantum systems ” . In : *Decision and Control (CDC), 2013 IEEE 52nd Annual Conference on*. Déc. 2013, p. 3714–3719. doi : 10.1109/CDC.2013.6760455. url : http://hal.archives-ouvertes.fr/hal-00800548/PDF/BVefficiency09.pdf.

I.2

Framework

This section describes some of the objects and tools that appear in my work. For instance I present

- the Dirac operator;
- the Maxwell equation.

I have also analysed the well known Schrödinger equation but my point of view was abstract and the properties I use are really well known. I did not think it was useful to describe them.

I included a description of the commutator methods as they are important in my work. I also added two appendices. The first is a brief description of the spectral theory concepts that I use and the second is some unpublished detailed proof of the Mourre method including the treatment of high energies.

For familiar reader, this chapter can be skipped. In the rest of the manuscript we will refer precisely to what is needed.

2.1 The Dirac operator

2.1.1 Some physical motivation

The Dirac equation models the motion of a quantum relativistic electron. Hence from the evolution principle of quantum mechanics, it is of the form:

$$\mathrm{i}\partial_t\psi(t) = H\psi(t)$$

where ψ is in a Hilbert space $\mathcal{H}$ (superposition principle) and H is a self-adjoint operator on $\mathcal{H}$ quantifying the energy (quantification principle).

For the free non-relativistic electron, the energy operator is obtained with the usual correspondence principle of Schrödinger:

$$\begin{aligned} P = -\mathrm{i}\nabla &\leftrightarrow p \\ Q &\leftrightarrow x \end{aligned}$$

applied to the classical energy[*]

$$E = \frac{mv^2}{2} + V(x) = \frac{p^2}{2m} + V(x) \text{ as } p = mv.$$

[*]Recall that p is the momentum, v the velocity and x the position in classical mechanics.

It takes the form

$$H = \frac{P^2}{2m} + V(Q) = \frac{-\Delta}{2m} + V(Q)$$

where $V(Q)$ denotes the operator of multiplication by V that is

$$(V(Q)\psi)(x) = V(x)\psi(x).$$

This gives the famous Schrödinger equation.

The energy given by the special relativity satisfies:

$$E^2 = c^2p^2 + m^2c^4.$$

We fix units such that the speed of light c is 1. Using Schrödinger's principle, we can obtain H the Dirac operator:

- The first idea could be the relativistic Schrödinger operator

  $$H = \sqrt{-\Delta + m^2},$$

  defined with the Fourier transform. But this operator is not local and in the associated equation, an asymmetry between time and spatial derivations appears and violates relativistic principles.

- P.A.M. Dirac proposed, in 1928, an operator linear with respect to $P = -\mathrm{i}\nabla$:

  $$D_m = \sum_{j=1}^{3} \alpha_j(-\mathrm{i}\nabla_j) + m\beta,$$

  such that $D_m^2 = -\Delta + m^2$. If $m \neq 0$, this imposes the relations

  $$\begin{cases} \alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij} \\ \beta\alpha_i + \alpha_i\beta = 0 \\ \beta^2 = 1. \end{cases}$$

  The ambient Hilbert space is thus $L^2(\mathbb{R}^3, \mathbb{C}^4) \equiv L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$, it makes appear two sets of degrees of freedom:

  1. The spin that is the intrinsic magnetic momentum of the electron which is thus a natural relativistic quantity;
  2. The sign of the energy.

The spectrum of D_m is $(-\infty, -m] \cup [+m, +\infty)$. The interpretation, given by Dirac, of the negative part of the spectrum has important physical consequences such as the prediction of the antiparticle of the electron: the positron.

Unfortunately, the classical theory introduced by Dirac does not allow the creation or annihilation of particles. For this one should consider, instead of classical functions, trace class operators. Nonetheless and despite of this strong indefiniteness, this operator can be used to model different type of phenomenon. The ones we have in mind are of non-linear interaction type as phenomenological models for self-interacting extended particles (one can find an interesting account of the possible models in [Ran]).

2.1.2 Definition

The free Dirac operator is hence usually defined as a differential operator acting on square integrable valued 4-spinors (vector of $L^2(\mathbb{R}^3, \mathbb{C})^{4\dagger}$). It is determined by the first order differential expression

$$D_m := \alpha \cdot P + m\beta = -\mathrm{i} \sum_{k=1}^{3} \alpha_k \partial_k + m\beta,$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, and the Pauli-Dirac matrices are:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} I_{\mathbb{C}^2} & 0 \\ 0 & -I_{\mathbb{C}^2} \end{pmatrix},$$

$$\text{for } \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We assume that the units are fixed so that $c = \hbar = 1$.

When the space dimension n is different from 3 then there exists N an integer such that D_m is the free Dirac operator acting on square integrable valued N-spinors of the form

$$D_m = -\mathrm{i}\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta m = \sum_{\jmath=1}^{n} -\mathrm{i}\alpha^\jmath \partial_{x_\jmath} + \beta m \qquad m > 0$$

where the $N \times N$ Dirac matrices are hermitian and satisfy

$$(\alpha^\jmath)^2 = \beta^2 = I_N, \qquad \alpha^\jmath \alpha^k + \alpha^k \alpha^\jmath = 2\delta_{\jmath k} I_N, \qquad \alpha^\jmath \beta + \beta \alpha^\jmath = 0, \qquad 1 \leq \jmath, k \leq n \quad (2.1)$$

where I_N is the $N \times N$ identity matrix. The integer N is even as from (2.1), each matrix coefficient is hermitian unitary and has zero trace.

As the Dirac matrices generate a faithful representation of the Clifford algebra over Minkowski spaces then for $n = 2d - 1$, odd dimensions, or $n = 2d$, even dimensions, they acts on spinors of dimension 2^{kd} for some $k \in \mathbb{N}$. Hence beside being even, N has to satisfy

$$N \in \left\{ 2^{k[\frac{n+1}{2}]}, k \in \mathbb{N} \right\}.$$

We refer to [KY01, Appendix], where the minimal N is proved to be $2^{[\frac{n+1}{2}]}$.

There are different possibilities for the matrices for instance the matrices can be swapped. But any choice is unitarily equivalent up to a time reversion as stated in the

Lemma 2.1 (Dirac–Pauli theorem). *Let $\{\alpha^\jmath,\ 1 \leq \jmath \leq n;\ \beta\}$ and $\{\tilde{\alpha}^\jmath,\ 1 \leq \jmath \leq n;\ \tilde{\beta}\}$, be two sets of the Dirac matrices of the same dimension N:*

$$\{\alpha^\jmath, \alpha^k\} = 2\delta_{\jmath k}, \quad \{\alpha^\jmath, \beta\} = 0; \qquad \{\tilde{\alpha}^\jmath, \tilde{\alpha}^k\} = 2\delta_{\jmath k}, \quad \{\tilde{\alpha}^\jmath, \tilde{\beta}\} = 0.$$

1. *Let $n = 2d - 1$, $d \in \mathbb{N}$. There is an invertible matrix S such that*

$$\tilde{\alpha}^\jmath = S^{-1} \alpha^\jmath S, \qquad 1 \leq \jmath \leq n; \qquad \tilde{\beta} = S^{-1} \beta S. \quad (2.2)$$

2. *Let $n = 2d$, $d \in \mathbb{N}$. There is an invertible matrix S and $\sigma \in \{\pm 1\}$ such that*

$$\tilde{\alpha}^\jmath = S^{-1} \alpha^\jmath S, \qquad 1 \leq \jmath \leq n-1; \qquad \tilde{\alpha}^n = \sigma S^{-1} \alpha^n S; \qquad \tilde{\beta} = S^{-1} \beta S.$$

†We will identify $L^2(\mathbb{R}^3)^4$, $L^2(\mathbb{R}^3, \mathbb{C}^4)$ and $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$.

Since the matrices $\tilde{\alpha}$ are hermitian, by taking the adjoint we show that the matrix S^*S commutes to the matrices α so that we can eliminate $|S|$ and choose S to be unitary.

We refer to [Shi11; Shi13; Pau36; Wae74; Dir28] or [Tha92, Lemma 2.25] for proofs and also [Kes61, Theorem 7] for general version in odd spatial dimensions. We provided a sketch of the proof in [BC12, Lemma 4.5].

The Dirac operator is built in order to satisfy

$$D_m^2 = (-\Delta + m^2) I_N.$$

Standard arguments involving the Fourier transform show that D_m defines a self-adjoint operator with domain $H^1(\mathbb{R}^n)^N$ and that the spectrum of D_m is

$$\sigma(D_m) = (-\infty, -m] \cup [m, \infty).$$

2.1.3 Spherically symmetric potentials and radial reduction

Due to the matrix structure of the Dirac operator, the representation of the orthogonal group are not as simple as in the scalar case. For instance radially symmetric N-spinors are not left invariant by the Dirac operator and radially symmetric potentials have a particular matrix structure.

In the 3-dimensional case for the standard Dirac representation (2.2), we considered, among others, hermitian 4×4 matrix multiplication operators, V, acting on $L^2(\mathbb{R}^3)^4$, such that $\mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{0\})^4 \subset \mathrm{D}(V)$ and

$$e^{\mathrm{i}\varphi n \cdot S} V(R^{-1}x) e^{-\mathrm{i}\varphi n \cdot S} = V(x), \ \forall x \in \mathbb{R}^3, \ \forall \varphi \in [0, 4\pi),$$

where

$$S = \frac{1}{2} \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$$

is the spin operator, and R is the matrix of the rotation of angle φ and axis n.

Spherically symmetric potentials may be constructed from maps

$$\phi_{\mathrm{sc,el,am}} : \mathbb{R} \longrightarrow \mathbb{R}$$

via

$$V(x) = \phi_{\mathrm{sc}}(|x|)\beta + \phi_{\mathrm{el}}(|x|) I_{\mathbb{C}^4} + i\phi_{\mathrm{am}}(|x|)\beta\alpha \cdot \frac{x}{|x|}. \tag{2.3}$$

The subscripts "sc", "el" and "am", stand for "scalar", "electric" and "magnetic" potential, respectively. Radial symmetry on the electric potential, for instance, is a consequence of the assumption that the atomic nucleus is pointwise and the electric forces are isotropic in an isotropic medium like the vacuum. In the particular Coulomb case $\phi_{\mathrm{sc}} = \phi_{\mathrm{am}} = 0$ and $\phi_{\mathrm{el}}(r) = \gamma/r$, $\sqrt{3}/2 < \gamma < 0$, $D_m + V$ describes the motion of a relativistic electron in the field created by an atomic nucleus.

If we consider, for any $\Psi \in L^2(\mathbb{R}^3)^4$, the spherical coordinates representation:

$$\psi(r, \theta, \phi) = r\Psi(r \sin(\theta)\sin(\phi), r\sin(\theta)\cos(\phi), r\cos(\theta)) \tag{2.4}$$

where $(r, \theta, \phi) \in (0, \infty) \times [0, \pi) \times [-\pi, \pi)$. The map $\Psi \mapsto \psi$ is an isomorphism between $L^2(\mathbb{R}^3)^4$ and $L^2((0,\infty), dr) \otimes L^2(S^2)^4$.

Then $L^2(S^2)^4$ decomposes as the direct sum of the two-dimensional angular momentum subspaces $\mathfrak{K}_{m_j,\kappa_j}$ (see [Tha92, Section 4.6]), the partial wave subspaces are given by

$$\mathfrak{H}_{m_j,\kappa_j} = L^2((0,\infty), dr) \otimes \mathfrak{K}_{m_j,\kappa_j},$$

so that $L^2(\mathbb{R}^3)^4 = \bigoplus \mathfrak{H}_{m_j,\kappa_j}$. The indices (m_j, κ_j) run over the set $m_j \in \{-j, \cdots, j\}$ and $\kappa_j \in \{\pm(j+\frac{1}{2})\}$, for $j \in \{\frac{2k+1}{2} : k \in \mathbb{N}\}$.

The r factor in (2.4) renders a Dirichlet boundary condition at 0. The dense subspaces $C_0^\infty(0,\infty) \otimes \mathfrak{K}_{m_j,\kappa_j} \subset \mathfrak{H}_{m_j,\kappa_j}$ are invariant under the action of H. If V is as in (2.3), then $H \restriction C_0^\infty(0,\infty) \otimes \mathfrak{K}_{m_j,\kappa_j}$ is unitary equivalent to

$$H_{m_j,\kappa_j} := \begin{pmatrix} 1 + \phi_{\mathrm{sc}}(r) + \phi_{\mathrm{el}}(r) & -\frac{d}{dr} + \frac{\kappa_j}{r} + \phi_{\mathrm{am}}(r) \\ \frac{d}{dr} + \frac{\kappa_j}{r} + \phi_{\mathrm{am}}(r) & -1 - \phi_{\mathrm{sc}}(r) + \phi_{\mathrm{el}}(r) \end{pmatrix}. \tag{2.5}$$

The operators H_{m_j,κ_j} are essentially self-adjoint in $C_0^\infty(0,\infty)^2$ under suitable conditions on the potentials $\phi_{\mathrm{sc,el,am}}$. Then one has

$$\sigma(H) = \overline{\bigcup \sigma(H_{m_j,\kappa_j})}.$$

The sub-index (m_j, κ_j) are often suppressed from operators and spaces, and only the index $\kappa \equiv \kappa_j$ is written. Note that the eigenvalues of H are degenerate and their multiplicity is at least m_j. We have

$$\sigma_{\mathrm{disc}}(H) = \bigcup \sigma_{\mathrm{disc}}(H_\kappa).$$

We have $\sigma_{\mathrm{ess}}(H_\kappa) = (-\infty, -1] \cup [1, \infty)$, so that H_κ are strongly indefinite as well.

In any dimension, referring to [KY01], we have

$$\alpha \cdot P = \alpha_r \left(p_r + \frac{\mathrm{i}}{r} K \right)$$

where

$$\alpha_r := \alpha \cdot \frac{x}{r}, \quad p_r := -\mathrm{i} r^{-\frac{n-1}{2}} \partial_r r^{\frac{n-1}{2}} = -\mathrm{i} \left(\partial - r + \frac{n-1}{2r} \right)$$

and

$$K := \frac{n-1}{2} - \sum_{1 \le j < k \le n} i\alpha_j \alpha_k (x_j P_k - x_k P_j)$$

is the spin-orbit coupling operator. Its self-adjoint extension on $L^2(S^{n-1})$ has purely discrete spectrum

$$-(\mathbb{N} + \frac{n-3}{2}) \cup (\mathbb{N} + \frac{n-3}{2}).$$

The Dirac operator in n-dimensions acts invariantly in each of the sum

$$\mathcal{E}_\kappa := L^2((0,\infty), r^{-\frac{n-1}{2}}\, dr) \otimes (\langle \phi \rangle \oplus \langle \alpha_r \phi \rangle)$$

where $\phi \in \mathrm{Ker}(S - \kappa)$. For spherically symmetric potentials of the form

$$V(x) = \phi_{\mathrm{sc}}(|x|)\beta + \phi_{\mathrm{el}}(|x|) I_{\mathbb{C}^N} + \mathrm{i}\phi_{\mathrm{am}}(|x|)\beta\alpha_r$$

the same is true for $H := D_m + V$ the action of H on $\mathcal{E}_\kappa$ reads as (2.5).

2.1.4 The ground state of Dirac Coulomb operators

In dimension n larger than 3, when V is the Coulomb potential: $\phi_{\rm sc} = \phi_{\rm am} = 0$, $\phi_{\rm el}(r) = \gamma/r$ with, see [Tha92, Lemma 4.15, Theorem 4.16, Example 4.17],

$$-\sqrt{n(n-2)}/2 < \gamma < 0.$$

The eigenvalues of H_κ are given explicitly by

$$E_j = m\left(1 + \frac{\gamma^2}{(j+\sqrt{\kappa^2-\gamma^2})^2}\right)^{-1/2}.$$

Note that $E_j \to m$ as $j \to \infty$ for all values of κ. The ground state in dimension 3 of the full coulombic Dirac operator H is achieved when $\kappa = -1$ and $j = 0$. The first component in the radial reduction of the associated eigenfunction is given by:

$$u_0(r) = \nu_0\left(\frac{\gamma}{(1-\gamma^2)^{1/2}-1}\right) r^{\sqrt{1-\gamma^2}} e^{-(\gamma E_0/\sqrt{1-\gamma^2})r},$$

ν_0 is chosen so that $\|u_0\| = 1$.

2.1.5 The multicenter potential

We considered, in dimension $n = 3$ only, the following operator

$$H_\gamma := D_m + \gamma V_c, \text{ where } V_c := v_c \otimes \mathrm{Id}_{\mathbb{C}^N} \text{ and } v_c(x) := \sum_{k=1,\dots,n} \frac{z_i}{|x-a_i|}, \tag{2.6}$$

acting on $\mathcal{C}_c^\infty(\mathbb{R}^3 \setminus \{a_i\}_{i=1,\dots,n}; \mathbb{C}^N)$, with $a_i \neq a_j$ for $i \neq j$. The $\gamma \in \mathbb{R}$ is the coupling constant. The index c stands for *coulombic multi-centre*. Assuming

$$Z := |\gamma| \max_{i=1,\dots,n}(|z_i|) < \sqrt{3}/2, \tag{2.7}$$

the theorem of Levitan-Otelbaev[‡] ensures that H_γ is essentially self-adjoint and its domain is the Sobolev space $H^1(\mathbb{R}^3; \mathbb{C}^N)$, see [AY82; Kal98; Kla80; LR79; LRK80; LO77] for various generalizations. This condition corresponds to the nuclear charge $\alpha_{\rm at}^{-1} Z \leq 118$, where $\alpha_{\rm at}^{-1} = 137.035999710(96)$. Note that using the Hardy-inequality, the Kato-Rellich theorem will apply till $Z < 1/2$ and is optimal in the matrix-valued case, see [Tha92][Section 4.3] for instance. For $Z < 1$, one shows there exists only one self-adjoint extension so that its domain is included in $H^{1/2}(\mathbb{R}^3; \mathbb{C}^N)$, see [Nen75]. This covers the nuclear charges up to $Z = 137$. When $n = 1$ and $Z = 1$, this property still holds true, see [EL07]. Surprisingly enough, when $n = 1$ and $Z > 1$, there is no self-adjoint extension with domain included in $H^{1/2}(\mathbb{R}^3; \mathbb{C}^N)$, see [Xia99][Theorem 6.3].

In [Nen75], one shows for $Z < 1$ that the essential spectrum is given by $(-\infty, -m] \cap [m, \infty)$ for all self-adjoint extension.

2.1.6 A link with the Klein-Gordon equation

The identity

$$(\mathrm{i}\partial_t - D_0 - m\beta)(\mathrm{i}\partial_t + D_0 + m\beta) = (\Delta - m^2 - \partial_{tt}^2) I_N$$

[‡]From [Che77, Theorem 2.1] and Section 2.1.4, we deduce the same result.

shows the intimate relation between the Dirac and the Klein-Gordon equation with mass m^2 (the wave equation if $m = 0$).

It is a way to derive properties of the free Dirac flow from the corresponding ones for the scalar Klein-Gordon and Wave equations using these identities.

For general self-adjoint perturbations H (of the Dirac operator), the *squared* Dirac equation

$$(\mathrm{i}\partial_t - H)(\mathrm{i}\partial_t + H) = (-\partial_{tt} - H^2)$$

can also be considered as a Klein-Gordon type equation.

2.2 The Maxwell operator

The physical phenomenon of electromagnetic oscillations in a resonator filled with a homogeneous medium is described by the isotropic Maxwell eigenvalue problem,

$$\begin{cases} \operatorname{curl} \boldsymbol{E} = \mathrm{i}\omega \boldsymbol{H} & \text{in } \Omega \\ \operatorname{curl} \boldsymbol{H} = -\mathrm{i}\omega \boldsymbol{E} & \text{in } \Omega \\ \boldsymbol{E} \times \mathbf{n} = 0 & \text{on } \partial\Omega, \end{cases} \tag{2.8}$$

where the angular frequency ω is a real and the field phasor $(\boldsymbol{E}, \boldsymbol{H}) \neq 0$ is restricted to the solenoidal subspace, characterised by the Gauss law

$$\operatorname{div}(\boldsymbol{E}) = 0 = \operatorname{div}(\boldsymbol{H}).$$

The orthogonal complement of this subspace is the gradient space, which is in the kernel of (2.8). The permittivities we considered are such that

$$\epsilon,\ \frac{1}{\epsilon},\ \mu,\ \frac{1}{\mu} \in L^\infty(\Omega). \tag{2.9}$$

In order to give a meaning to the normal to the boundary, it is usual to impose some regularity in the domain. Actually one can avoid such an assumption by imposing directly some symmetry on the associated operator. In this respect, we follow closely [BS90], the self-adjoint Maxwell operator has domain defined as follows. Consider

$$\mathcal{H}(\operatorname{curl};\Omega) = \left\{\boldsymbol{u} \in L^2(\Omega)^3 : \operatorname{curl} \boldsymbol{u} \in L^2(\Omega)^3\right\}$$
$$\mathcal{H}_0(\operatorname{curl};\Omega) = \{\boldsymbol{u} \in \mathcal{H}(\operatorname{curl};\Omega) : \int_\Omega \operatorname{curl} \boldsymbol{u} \cdot \boldsymbol{v} = \int_\Omega \boldsymbol{u} \cdot \operatorname{curl} \boldsymbol{v} \quad \forall \boldsymbol{v} \in \mathcal{H}(\operatorname{curl};\Omega)\}.$$

The linear space $\mathcal{H}(\operatorname{curl};\Omega)$ becomes a Hilbert space for the norm

$$\|\boldsymbol{u}\|_{\operatorname{curl},\Omega} = \left(\|\boldsymbol{u}\|_{0,\Omega}^2 + \|\operatorname{curl} \boldsymbol{u}\|_{0,\Omega}^2\right)^{1/2},$$

where

$$\|\boldsymbol{v}\|_{0,\Omega} = \left(\int_\Omega |\boldsymbol{v}|^2\right)^{1/2}$$

is the corresponding norm of $L^2(\Omega)^3$. Moreover, we have

$$\mathcal{H}_0(\operatorname{curl};\Omega)^3 = \overline{C_0^\infty(\Omega)^3},$$

where the closure is in the norm $\|\cdot\|_{\operatorname{curl},\Omega}$.

By virtue of Green's identity for the rotational [GR86, Theorem I.2.11], if Ω is a Lipschitz domain [Amr+98, Notation 2.1], then $\boldsymbol{u} \in \mathcal{H}_0(\text{curl};\Omega)$ if and only if $\boldsymbol{u} \in \mathcal{H}(\text{curl};\Omega)$ and $\boldsymbol{u} \times \mathbf{n} = \mathbf{0}$ on $\partial\Omega$.

A domain of self-adjointness of the operator associated to (2.8) for $\epsilon = \mu = 1$ is

$$\mathcal{D}_1 = \mathcal{H}_0(\text{curl};\Omega) \times \mathcal{H}(\text{curl};\Omega) \subset L^2(\Omega)^6$$

and its action is given by

$$\mathcal{M}_1 = \begin{bmatrix} 0 & i\,\text{curl} \\ -i\,\text{curl} & 0 \end{bmatrix} : \mathcal{D}_1 \longrightarrow L^2(\Omega)^6.$$

For

$$\mathcal{P} = \begin{bmatrix} \epsilon^{1/2} I_{3\times 3} & 0 \\ 0 & \mu^{1/2} I_{3\times 3} \end{bmatrix},$$

condition (2.9) ensures that $\mathcal{P} : L^2(\Omega)^6 \longrightarrow L^2(\Omega)^6$ is bounded and invertible. Moreover,

$$\left(\omega, \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix}\right) \in \mathbb{R} \times \mathcal{D}_1$$

is a solution of (2.8), if and only if

$$\begin{bmatrix} \tilde{\boldsymbol{E}} \\ \tilde{\boldsymbol{H}} \end{bmatrix} = \mathcal{P} \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix}$$

is a solution of

$$\mathcal{P}^{-1}\mathcal{M}_1\mathcal{P}^{-1} \begin{bmatrix} \tilde{\boldsymbol{E}} \\ \tilde{\boldsymbol{H}} \end{bmatrix} = \omega \begin{bmatrix} \tilde{\boldsymbol{E}} \\ \tilde{\boldsymbol{H}} \end{bmatrix}.$$

Therefore $\mathcal{M} = \mathcal{P}^{-1}\mathcal{M}_1\mathcal{P}^{-1}$ on $\mathrm{D}(\mathcal{M}) = \mathcal{P}\mathcal{D}_1$ is the self-adjoint operator associated to (2.8).

As $\mathcal{M}$ anticommutes with complex conjugation, the spectrum is symmetric with respect to 0. Moreover, $\mathrm{Ker}(\mathcal{M})$ is infinite dimensional, because it always contains the gradient space, see [BS90].

Isotropic cylindrical symmetries. If $\Omega = \tilde{\Omega} \times (0,\pi)$ for $\tilde{\Omega} \subset \mathbb{R}^2$ an open simply connected set, then (2.8) decouples by separating the variables for $\epsilon = \mu = 1$. In turns, a non-zero ω is an eigenvalue of $\mathcal{M}_1$, if and only if either $\omega^2 = \lambda^2$ where λ^2 is a Dirichlet eigenvalue of the Laplacian in $\tilde{\Omega}$, or $\omega^2 = \nu^2 + \rho^2$ where ν^2 is a non-zero Neumann eigenvalue of the Laplacian in $\tilde{\Omega}$ and $\rho \in \mathbb{N}$.

The Neumann problem can be re-written as ($\nu = \omega$)

$$\begin{cases} \text{curl}\,\boldsymbol{E} = \mathrm{i}\omega H \\ \text{curl}\,H = -\mathrm{i}\omega\boldsymbol{E} \end{cases} \text{in } \tilde{\Omega} \qquad \boldsymbol{E}\cdot\mathbf{t} = \mathbf{0} \quad \text{on } \partial\tilde{\Omega}, \tag{2.10}$$

for

$$\left(\omega, \begin{bmatrix} \boldsymbol{E} \\ H \end{bmatrix}\right) \in \mathbb{R} \times (\tilde{\mathcal{D}}_1 \setminus \{0\}).$$

Here

$$\boldsymbol{E} = \begin{bmatrix} E_1 \\ E_2 \end{bmatrix}, \qquad \text{curl}\,\boldsymbol{E} = \partial_x E_2 - \partial_y E_1, \qquad \text{curl}\,H = \begin{bmatrix} \partial_y H \\ -\partial_x H \end{bmatrix},$$

$\mathbf{t}$ is the unit tangent to $\partial\tilde{\Omega}$ and

$$\tilde{\mathcal{D}}_1 = \left\{\boldsymbol{u} \in L^2(\Omega)^2 : \text{curl}\,\boldsymbol{u} \in L^2(\Omega) \text{ and } \boldsymbol{u}\cdot\mathbf{t} = \mathbf{0}\right\} \times \left\{u \in L^2(\Omega) : \text{curl}\,u \in L^2(\Omega)^2\right\}.$$

This defines the Maxwell equation and operator in the bi-dimensional setting.

2.3 Commutator methods

In this section, we describe commutator methods. Unlike the other sections, the operator of interest is now denoted H and not A. This may look inconsistent but A in these theories stands for the so-called conjugate operator.

The idea, which goes back to C.R. Putnam [Put67], is to use some auxiliary operator A to analyse the spectral properties of some operator H. This is for instance the case when one tries to analyse properties of the point spectrum by means of Virial methods, also called Pohozaev methods. In what we describe below, we were more interested on the properties of the essential spectrum.

For instance in [Put67], if H is a self-adjoint operator acting in a Hilbert space $\mathcal{H}$, one supposes that there is a *bounded* operator A so that

$$C := [H, \mathrm{i}A] > 0,$$

where "$>$" means non-negative and injective. The commutator has to be understood in the form sense:

$$\langle \psi, [H, \mathrm{i}A]\psi\rangle = \mathrm{i}\,\langle H\psi, A\psi\rangle - \mathrm{i}\,\langle A\psi, H\psi\rangle \quad \forall \psi \in D(H).$$

When it extends into a bounded operator between some spaces, we denote this extension $[H, \mathrm{i}A]$ as well. The operator A is said to be *conjugate* to H.

One deduces some estimates, namely the so called *Limiting Absorption Principle* (LAP), on the imaginary part of the resolvent, i.e., one finds some *weight* B, a closed injective operator with dense domain, so that

$$\sup_{\Re(z)\in\mathbb{R}, \Im(z)>0} \Im\langle f, (H-z)^{-1} f\rangle \leq \|Bf\|^2$$

see for instance [RS79, Theorem XIII.28]. This estimation is equivalent to the global propagation estimate, c.f. [Kat66] and [RS79][Theorem XIII.25]:

$$\int_{\mathbb{R}} \|B^{-1}e^{\mathrm{i}tH}f\|^2 dt \leq 2\|f\|^2 \tag{2.11}$$

This equivalence explains the recent increasing interest to commutator methods in the analysis of dispersive equations even though they go back to the late seventies.

The last estimates called Kato smoothness estimates or, for short, Kato estimates are similar to the classical Strichartz estimates. We can also mention that Kato smoothness estimates can be simpler to prove than Strichartz estimates in a perturbation framework. Indeed, one only needs an estimate on the resolvent.

Combining the knowledge of Strichartz in some "free case", a Duhamel formula linking this "free case" and the "perturbed case" and the Kato smoothness in this "perturbed case", we can deduce Strichartz estimates in the short range case, see [RS04, Section 4].

To close our comment on the use of commutator methods to establish estimates of the form (2.11), we can also mention that Morawetz estimates are in a sense of the form of (2.11) and are based on Virial identities, that are commutator methods.

At the spectral level, one infers that the spectrum of H is purely absolutely continuous with respect to the Lebesgue measure. In particular, H has no eigenvalue. To deal with the presence of eigenvalues, the fact that A is unbounded and with the 3-body-problem, E. Mourre has the idea to localise in energy the estimates and to allow a compact perturbation, see [Mou81]. With further hypotheses, one shows an estimate of the resolvent (and not only on the imaginary part[§]). The theory was finally improved in many directions and optimised in many ways, see [ABG96] for a more thorough discussion of these matters. We mention also [GGM04; GJ07; Gér08] for recent developments. We refer to Appendix B where we give a detailed proof and description of Mourre's method.

As we were concerned about thresholds, Mourre's method was not sufficient, as the estimate of the resolvent is given on an interval excluding thresholds. In [BM97] one generalizes the result of Putnam's approach. Under some conditions, one allows A to be unbounded. By asking some positivity on the Virial of the potential, one is able to conciliate the estimation of the resolvent above the threshold energy and the accumulation of eigenvalues under it.

[§]This property was called supersmoothness in [KY89].

Appendices to part I

I.A

The spectrum of a self-adjoint operator

In this section, we recall some facts from spectral theory.

A.1 Spectrum

Recall that a linear operator on a normed space B is the coupled data $(A, D(A))$ where $D(A)$ is a subspace of B and A a linear operator from $D(A)$ to B. To simplify the notation we often write A instead and refer to $D(A)$ as the domain of A. An operator A' is an extension of A if $D(A) \subset D(A')$ and $A' = A$ on $D(A)$. We will write $A \subset A'$.

An operator is densely defined if its domain is dense.

Definition A.1. *Let B be a Banach space. A linear operator $A\colon D(A) \subset B \to B$ is said to be closed if for every sequence $\{x_n\}_{n\in\mathbb{N}}$ in $D(A)$ converging to $x \in B$ such that $Ax_n \xrightarrow[n\to\infty]{} y \in B$, then $x \in D(A)$ and $Ax = y$. Equivalently, A is closed if its graph is closed in $B \times B$.*

For an operator A, if the closure of its graph in $B \times B$ is the graph of some operator, we call that operator the closure of A, and we say that A is closable. We denote the closure of A by $\overline{A}$. It follows that A is the restriction of $\overline{A}$ to $D(A)$.

A core of a closable operator is a subset C of $D(A)$ such that the closure of the restriction of A to C, or the closure of $(A\restriction_C, C)$, is $(\overline{A}, D(\overline{A}))$.

A core is also a dense subspace for the graph topology, namely the space $D(A)$ endowed with the norm

$$u \mapsto \|u\| + \|Au\|.$$

The following are immediate:

- Any bounded linear operator defined on the whole space B is closed. Notice that from the closed graph theorem, closed operator A with $D(A) = B$ are exactly bounded operators on B;
- An operator A admits a closure if and only if for every sequence $\{x_n\}$ converging to 0 in B, and such that $\{Ax_n\}$ converges to v in B, then $v = 0$.

For simplicity we replace the Banach space B by a Hilbert space $\mathcal{H}$. If A is a densely defined operator, we define its adjoint A^* by

$$D(A^*) = \{\phi \in \mathcal{H}, \text{s.t. } \exists \eta \in \mathcal{H}, \forall \psi \in D(A), \langle \phi, A\psi\rangle = \langle \eta, \psi\rangle\}$$

and for any $\phi \in D(A^*)$, $A^*\phi = \eta$. The uniqueness of η follows from the density of the domain of A.

Using transformation $(\psi, \eta) \mapsto (-\eta, \psi)$ in $\mathcal{H} \times \mathcal{H}$, Riesz lemma and Closed Graph theorem we deduce that A^* is closed and A is closable if and only if $D(A^*)$ is dense, [RS80, Theorem VIII.1].

Notice that if $A \subset A'$ then $(A')^* \subset A^*$.

Definition A.2. *A densely defined linear operator $A\colon D(A) \subset \mathcal{H} \to \mathcal{H}$ on a Hilbert space $\mathcal{H}$ is a hermitian or symmetric operator if $(A\psi, \phi) = (\psi, A\phi)$ for all $\psi, \phi \in D(A)$. This means that $A \subset A^*$.*

The operator A is self-adjoint if it coincides with its adjoint, i.e. if $A = A^*$. Notice that a symmetric operator is always closable and if its closure coincides with its adjoint (i.e. $\overline{A} = A^*$), then A is said to be essentially self-adjoint.

Definition A.3 (The spectrum of a self-adjoint operator)**.** *Let $A\colon D(A) \subset \mathcal{H} \to \mathcal{H}$ self-ajoint operator on a Hilbert space $\mathcal{H}$*

*The spectrum of A, usually denoted $\sigma(A)$, is the set of all complex numbers λ such that**

$$\lambda I_{\mathcal{H}} - A$$

is not invertible from $D(A)$ to $\mathcal{H}$.

The discrete spectrum is the set of eigenvalues isolated in $\sigma(A)$ and of finite multiplicity. Its complementary in the spectrum is the essential spectrum of A, denoted $\sigma_{\text{ess}}(A)$.

A complex number λ is in the resolvent set $\rho(A)$ of A if $A - \lambda I_{\mathcal{H}}$ is invertible (with bounded inverse) from $D(A)$ to $\mathcal{H}$. This is the complementary set of $\sigma(A)$. From

$$\|(A - zI_{\mathcal{H}})\psi\|^2 = \|(A + \Im z I_{\mathcal{H}})\psi\|^2 + |\Re z|^2 \|\psi\|^2, \tag{A.1}$$

we deduce the

Lemma A.4. *If A is self-adjoint, the spectrum is contained on the real axis. The essential spectrum is always closed, and it is a subset of the spectrum $\sigma(A)$.*

The following lemma explains why it is called the ”essential” spectrum.

Proposition A.5. *The essential spectrum is invariant under compact perturbations. That is, if K is a compact operator on $\mathcal{H}$, then the essential spectra of A and that of $A + K$ coincide.*

These different notions of spectrum can be extended to closed operators but for self-adjoint operators the essential spectrum can be characterised by many ways. Another characterisation that is useful is given by

Theorem A.6 (Weyl's characterisation)**.** *A number λ is in the spectrum of A if and only if there exists a sequence $\{\psi_k\}$ in the space $\mathcal{H}$ such that $||\psi_k|| = 1$ and*

$$\lim_{k\to\infty} |A\psi_k - \lambda\psi_k| = 0.$$

Furthermore, λ is in the essential spectrum if there is a sequence satisfying this condition, but such that it contains no convergent subsequence; such a sequence is called a singular sequence or Weyl sequence. For instance we can choose $\psi_k \to 0$ weakly.

*We often write $\lambda - A$ instead of $\lambda I_{\mathcal{H}} - A$.

A.2 Resolvent & functional calculus

If A is a self-adjoint operator acting on a Hilbert space $\mathcal{H}$, for any $\lambda \in \rho(A)$, the operator $R_A(\lambda) := (A - \lambda I_{\mathcal{H}})^{-1}$ is a bounded operator. Moreover for $\lambda, \lambda' \in \rho(A)$, $R_A(\lambda)$ commutes to $R_A(\lambda')$ and we have the following resolvent identity

$$R_A(\lambda) - R_A(\lambda') = (\lambda - \lambda')R_A(\lambda)R_A(\lambda').$$

Thus for $\lambda' \neq \lambda$ in the resolvent set of A, we have

$$I_{\mathcal{H}} = (\lambda' - \lambda)(I_{\mathcal{H}} - (\lambda - \lambda')R_A(\lambda'))\left((\lambda' - \lambda)^{-1}I_{\mathcal{H}} - R_A(\lambda)\right)$$

from which we deduce that the spectrum of $R_A(\lambda)$ is the closure of the image of the spectrum of A by $\lambda' \mapsto (\lambda' - \lambda)^{-1}$.

Consider Φ_A that maps the function $x \in \mathbb{R} \mapsto (x - z)^{-1}$ to $R_A(z)$. It extends to a unitary $*$-algebra morphism that maps bounded rational functions to bounded operator still denoted Φ_A. We can prove that if f is a non-negative bounded rational function then $\Phi_A(f)$ is non negative. This allows the extension of the map Φ_A to continuous functions tending to 0 at infinity, the class $C_0(\mathbb{R})$, with the property

$$\|\Phi_A(f)\| \leq \|f\|_\infty.$$

As this extension preserves the positivity, the functional Λ_ψ, for any $\psi \in \mathcal{H}$ defined by

$$f \in C_0(\mathbb{R}) \mapsto \langle u, \Phi_A(f)u\rangle$$

is a positive bounded functional. It is represented by a positive finite Borel measure and thus extends to any bounded borelian function f, allowing the extension of Φ_A with all the mentioned properties preserved. Thus we can obtain, see [RS80, Theorem VIII.5], the

Theorem A.7. *Let A be self-adjoint operator on $\mathcal{H}$. Then there exists a unique map Φ_A from the bounded Borel functions on $\mathbb{R}$ into $B(\mathcal{H})$ the space of bounded operators on $\mathcal{H}$ so that*

1. *Φ_A is an algebraic $*$-homomorphism*
2. *Φ_A is norm continuous, that is*
$$\|\Phi_A(f)\|_{B(\mathcal{H})} \leq \|f\|_\infty$$
3. *Let $(f_n)_{n\in\mathbb{N}}$ be a uniformly bounded sequence of bounded borelian functions converging pointwise to f then f is a borelian bounded function and*
$$\Phi_A(f_n)\psi \to \Phi_A(f)\psi \text{ in } \mathcal{H}.$$

In addition $\Phi_A(f) \geq 0$ when f is non-negative bounded borelian function.

Below we write $f(A)$ for $\Phi_A(f)$ for any bounded borelian function.

Compact resolvent. Riesz-Schauder theorem [RS80, Theorem VI.15] gives that if one of the resolvent of A is compact then the spectrum of A is made of isolated eigenvalues of finite algebraic multiplicity (the corresponding algebraic kernel is finite dimensional) possibly accumulating at infinity.

Notice that if one of the resolvent is compact then all of them are.

A.3 The min-max principle & Rayleigh-Ritz technique

The min-max characterisation of the lower part of the spectrum is given by

Theorem A.8. *If A is a self-adjoint operator on $\mathcal{H}$ bounded from below, $A \geq cI$ in the form sense for some $c \in \mathbb{R}$. Define*

$$\mu_n(A) = \sup_{\phi_1,\dots\phi_{n-1}} \inf_{\substack{\psi\in[\phi_1,\dots\phi_{n-1}]^\perp \\ \psi\in lD(A),\, \|\psi\|=1}} (\psi, A\psi)\,.$$

Then, for each n, either

(a) there are n eigenvalues (counting multiplicity) below the bottom of the essential spectrum, and $\mu_n(A)$ is the n-th eigenvalue counting multiplicity;

or

(b) $\mu_n(A)$ is the bottom of the essential spectrum, i.e., $\mu_n(A) = \inf\{\lambda\colon \sigma_{\mathrm{ess}}(A)\}$ and in this case $\mu_n(A) = \ldots = \mu_{n+k}(A) = \ldots$ an there are at most $n-1$ eigenvalues below $\mu_n(A)$.

We refer to Reed & Simon, [RS78, Chapter XIII] for more details. One important consequence of this theorem for numerical applications is the Rayleigh-Ritz technique, which shows that spectra of compressions provides upper bounds for the spectrum of operator bounded from below. This the content of the

Theorem A.9. *Let A be a self-adjoint semibounded operator on $\mathcal{H}$. Let $\mathcal{L}$ be an n-dimensional subspace of $D(A)$, and let P be the orthogonal projection onto $\mathcal{L}$. Let $A_{\mathcal{L}} = PA\restriction_{\mathcal{L}}$. Let $\mu_1^{\mathcal{L}} \leq \ldots \leq \mu_n^{\mathcal{L}}$ be the eigenvalues of $A_{\mathcal{L}}$. Then*

$$\mu_m(A) \leq \mu_m^{\mathcal{L}},\ m \in \{1,\ldots,n\}$$

The convergence of the so called Galerkin method in the case of operator which are bounded from below is a consequence of the

Theorem A.10 (XIII.4 Reed & Simon IV)**.** *Let A be a self-adjoint semibounded operator on $\mathcal{H}$. Let $(\mathcal{L}_n)_{n\in\mathbb{N}}$ be a sequence such that $\mathcal{L}_n$ is n-dimensional subspace of $D(A)$, and let P_n be the orthogonal projection onto $\mathcal{L}_n$.*

Suppose $\mu_1(A)$ is an eigenvalue of A with normalised eigenvector $\psi \in \overline{\cup_{n\in\mathbb{N}}\mathcal{L}_n}$. Suppose

$$\lim_{n\to\infty} (P_n\psi, AP_n\psi) = \mu_1(A).$$

Then

$$\lim_{n\to\infty} \mu_1^{\mathcal{L}_n} = \mu_1(A).$$

I.B

On the boundary values of the resolvent of a self-adjoint operator

In this appendix, we give detailed proofs of the main consequences of Mourre estimates on both bounded and unbounded intervals. Here again, the operator of interest is now denoted H and not A, which stands for the so-called conjugate operator.

We study a self-adjoint operator H in a Hilbert space $\mathcal{H}$ with the help of an auxiliary self-adjoint operator A.

B.1 The assumptions

We assume the following

Assumption B.1.1. *The unitary operators $W_\alpha = e^{i\alpha A}$, $\alpha \in \mathbb{R}$, leaves the domain $D(H)$ of H invariant. We write $H_\alpha = W_\alpha^* H W_\alpha$ considered as an operator from $D(H)$ to $\mathcal{H}$.*

Assumption B.1.2. *For all $u \in D(H)$ the function $\alpha \in \mathbb{R} \mapsto H_\alpha u \in \mathcal{H}$ is twice differentiable. We write $H'_\alpha u$ and $H''_\alpha u$ for its derivatives at the first and second order and we define two linear operators H' and H'' with domain $D(H)$ in $\mathcal{H}$ by $H'u = H'_0 u$ and $H''u = H''_0 u$.*

Assumption B.1.3. *There exists $J \subset \mathbb{R}$ an open interval such that there exist $a_0 > 0$ and a compact operator K in $\mathcal{H}$ such that :*

$$\mathbb{1}_J(H) H' \mathbb{1}_J(H) \geq a_0 \mathbb{1}_J(H) + K.$$

This last assumption is usually called Mourre estimate.

With no further mention, we consider these assumptions on each of the following statements.

B.2 On the discrete spectrum

Let $W_\alpha^\circ = W_\alpha \restriction_{D(H)}$ considered as an operator in $D(H)$. We have the

Lemma B.1. *The operators H' and H'' are bounded from $D(H)$ to $\mathcal{H}$ and symmetric.*

Proof – As an immediate consequence of the Banach-Steinhauss theorem, we obtain the boundedness.

The operator H is selfadjoint and $W_\alpha D(H) \subset W_\alpha$. Differentiating in α the identity $\langle u, H_\alpha v\rangle = \langle H_\alpha u, v\rangle$ for any u and v in $D(H)$ gives the symmetry. □

Lemma B.2. *For all real α, $W^\circ_\alpha \in B(D(H))$ and there exist M and ω in $\mathbb{R}$ such that for*

$$\|W^\circ_\alpha\|_{B(D(H))} \le Me^{\omega\alpha} \quad \forall \alpha \in \mathbb{R}.$$

Proof – To prove that $W^\circ_\alpha \in B(D(H))$, it is enough to prove that its graph is closed in $D(H) \times D(H)$. So if $(u_n)_{n\in\mathbb{N}}$ is such that $u_n \to u$, $Hu_n \to Hu$, $W_\alpha u_n \to v$ and $HW_\alpha u_n \to Hv$ then $v = W_\alpha u$ since W_α is a bounded operator on $\mathcal{H}$ and W°_α is bounded by the closed graph theorem.

By the previous lemma, H' is bounded from $D(H)$ to $\mathcal{H}$ and $H'_\alpha = W^*_\alpha H' W_\alpha$, so

$$HW^\circ_\alpha = H + \int_0^\alpha W^*_{\alpha-\beta} H' W_\beta \, d\beta$$

and thus

$$\|W^\circ_\alpha u\|_{D(H)} \le \|u\|_{D(H)} + C\int_0^\alpha \|W^\circ_\beta u\|_{D(H)} \, d\beta$$

so the lemma follows from Gronwall lemma. □

Lemma B.3 (Virial)**.** *For any eigenvector u of H, $\langle u, H'u\rangle = 0$.*

Proof – For any $u \in D(H)$, the map $f : \alpha \in \mathbb{R} \mapsto (H_\alpha - i)^{-1}u$ is differentiable at 0:

$$\frac{f(\alpha) - f(0)}{\alpha} = -(H_\alpha - i)^{-1}\frac{H_\alpha - H}{\alpha}(H - i)^{-1}u$$

tends to $-(H-i)^{-1}H'(H-i)^{-1}u$ due to the local uniform boundedness of $\alpha \to (H_\alpha - i)^{-1}$ (following from the above lemma) since $(H_\alpha - i)^{-1} = W^*_\alpha (H - i)^{-1} W_\alpha$. Hence we get $R(i)' = -R(i)H'R(i)$.

Then one has:

$$\frac{(H_\alpha - i)^{-1} - (H - i)^{-1}}{\alpha} = \frac{W^*_\alpha(H - i)^{-1}W_\alpha - (H - i)^{-1}}{\alpha}$$

or

$$\frac{(H_\alpha - i)^{-1} - (H - i)^{-1}}{\alpha} = \left\{\frac{W^*_\alpha - 1}{\alpha}(H - i)^{-1} - (H - i)^{-1}\frac{W^*_\alpha - 1}{\alpha}\right\} W_\alpha$$

and hence applying it to $W^*_\alpha u$ we obtain:

$$R(i)' = \lim_{\alpha\to 0}[\frac{W^*_\alpha - 1}{\alpha}, (H - i)^{-1}]u$$

so if u is an eigenvector (associated to an eigenvalue λ),

$$\langle u, [\frac{W^*_\alpha - 1}{\alpha}, (H - i)^{-1}]u\rangle = 0$$

and

$$\langle u, R(i)'u\rangle = 0$$

and finally

$$\langle (H - i)^{-1}u, H'(H - i)^{-1}u\rangle = 0$$

hence with $(H - i)^{-1}u = (\lambda - i)^{-1}u$ we obtain the lemma. □

Corollary B.4. *The interval J contains at most a finite number of eigenvalues, each of them of finite multiplicity.*

Proof – Assume the assertion if false, then there exist a sequence $(u_n)_{n\in\mathbb{N}}$ of orthonormal eigenvectors of H with eigenvalues in J, from the Mourre estimate and the previous lemma, we have :

$$a_0\langle u_n, u_n\rangle \leq -\langle u_n, Ku_n\rangle$$

Since $u_n \rightharpoonup 0$ weakly with $\|u_n\| = 1$ and K is compact, we obtain $a_0 \leq 0$, which is a contradiction. □

B.3 The limiting absorption principle

If the interval J does not contain any eigenvalue, we can get ride of K in the Mourre estimate:

Lemma B.5. *If $\lambda \in J$ is not an eigenvalue then, there exists $\nu_0 > 0$ and $a \in (0, a_0)$ such that for $J_\nu = (\lambda-\nu, \lambda+\nu)\cap J$*

$$\mathbb{1}_{J_\nu}(H)H'\mathbb{1}_{J_\nu}(H) \geq a\mathbb{1}_{J_\nu}(H) \quad \forall\nu \geq \nu_0.$$

Proof – Indeed, $\mathbb{1}_{J_\nu}(H) \to 0$ in the strong sense as $\nu \to 0$ hence $K\mathbb{1}_{J_\nu}(H) \to 0$ in the norm sense as $\nu \to 0$. □

We have a similar lemma for neighbourhood of infinity:

Lemma B.6. *There exists $\nu_0 > 0$ and $a \in (0, a_0)$ such that for $J_\nu = J \setminus (-1/\nu, 1/\nu)$*

$$\mathbb{1}_{J_\nu}(H)H'\mathbb{1}_{J_\nu}(H) \geq a\mathbb{1}_{J_\nu}(H) \quad \forall\nu \geq \nu_0.$$

Proof – Again, $\mathbb{1}_{J_\nu}(H) \to 0$ in the strong sense as $\nu \to +\infty$ hence $K\mathbb{1}_{J_\nu}(H) \to 0$ in the norm sense as $\nu \to +\infty$. □

In the following, J_ν will be one of the interval: $(\lambda-\nu, \lambda+\nu)\cap J$ or $J\setminus(-1/\nu, 1/\nu)$, which we assume to be non empty.

Lemma B.7. *For sufficiently small $\delta > 0$, there exists $c_\delta > 0$ positive such that for all $u \in D(H)$, for all $\nu \geq \nu_0$:*

$$(a-\delta)\|\mathbb{1}_{J_\nu}(H)u\|^2 \leq \langle H'u, u\rangle + c_\delta\|(1-\mathbb{1}_{J_\nu}(H))u\|_H^2.$$

Proof – From the previous lemmata, we have

$$\langle u, \mathbb{1}_{J_\nu}(H)H'\mathbb{1}_{J_\nu}(H)u\rangle \geq a\|\mathbb{1}_{J_\nu}(H)u\|^2.$$

so that

$$\begin{aligned}&\langle u, H'u\rangle\\ &\geq \langle(1-\mathbb{1}_{J_\nu}(H))u, H'(1-\mathbb{1}_{J_\nu}(H))u\rangle + 2\Re\langle H'(1-\mathbb{1}_{J_\nu}(H))u, \mathbb{1}_{J_\nu}(H)u\rangle + a\|\mathbb{1}_{J_\nu}(H)u\|^2.\end{aligned}$$

By Cauchy-Schwartz inequality, we have for some $C > 0$

$$\begin{aligned}&|\langle(1-\mathbb{1}_{J_\nu}(H))u, H'(1-\mathbb{1}_{J_\nu}(H))u\rangle|\\ &\leq \frac{1}{2}\|H'(1-\mathbb{1}_{J_\nu}(H))u\|^2 + \frac{1}{2}\|(1-\mathbb{1}_{J_\nu}(H))u\|^2 \leq C\|(1-\mathbb{1}_{J_\nu}(H))u\|_H^2\end{aligned}$$

and since $H' \in B(D(H), \mathcal{H})$

$$|\Re\langle H'(1 - \mathbb{1}_{J_\nu}(H))u, \mathbb{1}_{J_\nu}(H)u\rangle| \leq \frac{\delta}{2}\|\mathbb{1}_{J_\nu}(H)u\|^2 + \frac{1}{2\delta}\|H'(1 - \mathbb{1}_{J_\nu}(H))u\|^2$$

or

$$|\Re\langle H'(1 - \mathbb{1}_{J_\nu}(H))u, \mathbb{1}_{J_\nu}(H)u\rangle| \leq \frac{\delta}{2}\|\mathbb{1}_{J_\nu}(H)u\|^2 + \frac{\|H'R(i)\|}{2\delta}\|(1 - \mathbb{1}_{J_\nu}(H))u\|_H^2$$

So

$$\begin{aligned}\langle u, H'u\rangle \quad \geq \quad & -C\|(1 - \mathbb{1}_{J_\nu}(H))u\|_H^2 \\ & -\delta\|\mathbb{1}_{J_\nu}(H)u\|^2 - \frac{\|H'R(i)\|}{\delta}\|(1 - \mathbb{1}_{J_\nu}(H))u\|_H^2 \\ & +a\|\mathbb{1}_{J_\nu}(H)u\|^2.\end{aligned}$$

hence for a sufficiently small δ, we have the estimate. □

Lemma B.8. *Let $H_\epsilon = H - \mathrm{i}\epsilon H'$ for $\epsilon \in \mathbb{R}$ with domain $D(H_\epsilon) = D(H)$. For $|\epsilon| < \|H'R(i)\|^{-1}$, $H_\epsilon^* = H_{-\epsilon}$.*

Proof – We have from the symmetry of H and H' that $H_{-\epsilon} + \mathrm{i} \subset H_\epsilon^* + i$. From

$$H_\epsilon + i = (1 - i\epsilon H'(H + i)^{-1})(H + i)$$

and the fact that $H'(H + i)^{-1}$ is bounded, we deduce that for $|\epsilon| \leq \|H'R(i)\|^{-1}$, $H_\varepsilon + i$ is invertible and so $H_{-\epsilon} + i = H_\epsilon^* + i$ or $H_{-\epsilon} = H_\epsilon^*$ □

Lemma B.9. *There exists $C > 0$, such that for all $\lambda \in \mathbb{R}$, for all $\mu \in \mathbb{R}$, with $\mu\varepsilon \geq 0$, for all $u \in D(H)$, we have:*

$$|\epsilon + \mu|\|u\|^2 \leq C|\Im\langle(H_\varepsilon - \lambda - \mathrm{i}\mu)u, u\rangle| + C|\epsilon|\|(1 - \mathbb{1}_{J_\nu}(H))u\|_H^2.$$

Proof – From Lemma B.7, we have:

$$(a - \delta)\|\mathbb{1}_{J_\nu}(H)u\|^2 \leq \langle H'u, u\rangle + C\|(1 - \mathbb{1}_{J_\nu}(H))u\|_H^2 \quad \forall\nu \geq \nu_0$$

or

$$(a - \delta)|\varepsilon|\|\mathbb{1}_{J_\nu}(H)u\|^2 \leq \Im\langle i|\epsilon|H'u, u\rangle + |\varepsilon|C\|(1 - \mathbb{1}_{J_\nu}(H))u\|_H^2 \quad \forall\nu \geq \nu_0$$

and hence since $\mu\epsilon \geq 0$

$$(a - \delta)|\varepsilon + \mu|\|\mathbb{1}_{J_\nu}(H)u\|^2 \leq |\Im\langle(i\epsilon H' + i\mu)u, u\rangle| + |\varepsilon|C\|(1 - \mathbb{1}_{J_\nu}(H))u\|_H^2 \quad \forall\nu \geq \nu_0$$

and hence we obtain the desired estimate. □

Lemma B.10. *We have, for any $u \in D(H)$:*

$$\|(H_\epsilon - \lambda - \mathrm{i}\mu)u\|^2 \geq \langle u, \left[(H - \lambda)^2 - \|H'R(i)\||\epsilon|(1 + H^2)\right] u\rangle.$$

Proof – We have

$$\|(H_\epsilon - \lambda - \mathrm{i}\mu)u\|^2 = \|(H-\lambda)u\|^2 + \|(\epsilon H' + \mu)u\|^2 - 2\Re\langle (H-\lambda)u, i(\epsilon H' + \mu)u\rangle$$

or

$$\|(H_\epsilon - \lambda - \mathrm{i}\mu)u\|^2 = \|(H-\lambda)u\|^2 + \|(\epsilon H' + \mu)u\|^2 + 2\epsilon\Im\langle Hu, H'u\rangle.$$

Hence

$$\|(H_\epsilon - \lambda - \mathrm{i}\mu)u\|^2 \geq \|(H-\lambda)u\|^2 - 2|\epsilon|\|Hu\|\|H'u\|.$$

and so the result follows. □

The following results are the key estimate.

Lemma B.11 (bounded interval case)**.** *In the bounded case ($J_\nu = (\lambda_0 - \nu, \lambda_0 + \nu) \cap J$ for some $\lambda_0 \in J$) if $[\lambda - \eta, \lambda + \eta] \subset [\alpha, \beta] \subset J_\nu$ then*

$$\begin{aligned}&\|(H_\epsilon - \lambda - \mathrm{i}\mu)u\|^2 + (\epsilon + \epsilon^2)](|\lambda| + |\nu|)^2\|u\|^2 \\ &\geq \left[(1-\varepsilon)(\eta^2 \min(\frac{1}{1+\alpha^2}, \frac{1}{1+\beta^2}) - \|H'R(i)\||\epsilon|) - (\epsilon + \epsilon^2)\right] \|(1 - \mathbb{1}_{J_\nu}(H))u\|_H^2\end{aligned}$$

for any $u \in D(H)$.

Proof – We have

$$\begin{aligned}&\|(H_\epsilon - \lambda - \mathrm{i}\mu)(1 - \mathbb{1}_{J_\nu}(H))u\|^2 \\ &\geq \langle (1 - \mathbb{1}_{J_\nu}(H))u, \left[(H-\lambda)^2 - \|H'R(i)\||\epsilon|(1+H^2)\right](1 - \mathbb{1}_{J_\nu}(H))u\rangle\end{aligned}$$

and since

$$\begin{aligned}&\left[(H-\lambda)^2 - \|H'R(i)\||\epsilon|(1+H^2)\right](1 - \mathbb{1}_{J_\nu}(H)) \\ &\geq \left(\eta^2 \min(\frac{1}{1+\alpha^2}, \frac{1}{1+\beta^2}) - \|H'R(i)\||\epsilon|\right)(1+H^2)\end{aligned}$$

Then, we use

$$\begin{aligned}&\|(H_\epsilon - \lambda - \mathrm{i}\mu)u\|^2 \\ &= \|(H_\epsilon - \lambda - \mathrm{i}\mu)\mathbb{1}_{J_\nu}(H)u\|^2 + \|(H_\epsilon - \lambda - \mathrm{i}\mu)(1 - \mathbb{1}_{J_\nu}(H))u\|^2 \\ &\quad + 2\Re\langle (H_\epsilon - \lambda - \mathrm{i}\mu)(1 - \mathbb{1}_{J_\nu}(H))u, (H_\epsilon - \lambda - \mathrm{i}\mu)\mathbb{1}_{J_\nu}(H)u\rangle \\ &= \|(H_\epsilon - \lambda - \mathrm{i}\mu)\mathbb{1}_{J_\nu}(H)u\|^2 + \|(H_\epsilon - \lambda - \mathrm{i}\mu)(1 - \mathbb{1}_{J_\nu}(H))u\|^2 \\ &\quad - 2\epsilon\Im\langle (H - \lambda - \mathrm{i}\mu)(1 - \mathbb{1}_{J_\nu}(H))u, H'\mathbb{1}_{J_\nu}(H)u\rangle \\ &\quad + 2\epsilon\Im\langle H'(1 - \mathbb{1}_{J_\nu}(H))u, (H - \lambda - \mathrm{i}\mu)\mathbb{1}_{J_\nu}(H)u\rangle \\ &\quad + 2\epsilon^2\Re\langle H'(1 - \mathbb{1}_{J_\nu}(H))u, H'\mathbb{1}_{J_\nu}(H)u\rangle \\ &\geq (1-\epsilon)\|(H_\epsilon - \lambda - \mathrm{i}\mu)\mathbb{1}_{J_\nu}(H)u\|^2 + (1-\epsilon)\|(H_\epsilon - \lambda - \mathrm{i}\mu)(1 - \mathbb{1}_{J_\nu}(H))u\|^2 \\ &\quad - (\epsilon + \epsilon^2)\|H'\mathbb{1}_{J_\nu}(H)u\|^2 \\ &\quad - (\epsilon + \epsilon^2)\|H'(1 - \mathbb{1}_{J_\nu}(H))u\|^2 \\ &\geq (1-\epsilon)\|(H_\epsilon - \lambda - \mathrm{i}\mu)(1 - \mathbb{1}_{J_\nu}(H))u\|^2 \\ &\quad - (\epsilon + \epsilon^2)\|Hu\|^2\end{aligned}$$

to conclude. □

The unbounded case is immediate

Lemma B.12 (unbounded interval case). *In the unbounded case ($J_\nu = J \setminus (-1/\nu, 1/\nu)$) if $\lambda \in J_\nu$ then*

$$(1+\frac{1}{\nu^2})\|u\|^2 \geq \|(1-\mathbb{1}_{J_\nu}(H))u\|_H^2$$

for any $u \in D(H)$.

All the previous results gathers to obtain the following propositions.

Proposition B.13. *For $I \subset \mathbb{R}$ such that $\operatorname{dist}(I, J_\nu^c) \geq \eta$, for some positive η, there exist $\varepsilon_0 > 0$ and $C > 0$ such that*

$$\forall\epsilon \in (0,\epsilon_0),\ \forall\lambda \in I,\ \forall\mu \geq 0,\ \ (\epsilon+\mu)\|u\|^2 \leq C|\Im\langle(H_\varepsilon-\lambda-\mathrm{i}\mu)u,u\rangle|+C\epsilon\|(H_\varepsilon-\lambda-\mathrm{i}\mu)^{(*)}u\|^2$$

for any $u \in D(H)$.

Proposition B.14. *For $I \subset \mathbb{R}$ such that $I \subset J \cap [-\eta,\eta]^c$, for a sufficiently large η for all $\lambda \in I$, for all $\mu \geq 0$, $(H_\varepsilon - \lambda - \mathrm{i}\mu) : D(H) \to \mathcal{H}$ is invertible and its inverse R_ϵ satisfies*

$$(\epsilon+\mu)\|R_\epsilon^{(*)}f\|^2 \leq C|\Im\langle f, R_\varepsilon^{(*)}f\rangle| + C\epsilon\|f\|^2$$

for any $f \in \mathcal{H}$.

Proposition B.15. *For $F_\varepsilon = \langle f, R_\varepsilon f\rangle$, we have*

$$F'_\varepsilon = \frac{dF_\varepsilon}{d\varepsilon} = \langle R_\varepsilon^* f, Af\rangle - \langle Af, R_\varepsilon f\rangle - \varepsilon\langle R_\varepsilon^* f, H'' R_\varepsilon f\rangle$$

for any $f \in D(A)$.

Proof – For any $f \in D(A)$, a resolvent type identity gives

$$\frac{F_\varepsilon - F_{\varepsilon'}}{\varepsilon - \varepsilon'} = \langle R_\varepsilon^{(*)}f, H' R_{\varepsilon'} f\rangle$$

since $R_\varepsilon f \in D(H)$ and so

$$\frac{dF_\varepsilon}{d\varepsilon} = \mathrm{i}\langle R_\varepsilon^{(*)} f, H' R_\varepsilon f\rangle$$

In the other hand,

$$H'f = \lim_{\alpha\to 0}[\frac{W_\alpha^* - 1}{\alpha}, H]f$$

so plugging in the above identity, one gets taking the limit, one gets

$$\frac{dF_\varepsilon}{d\varepsilon} = \lim_{\alpha\to 0}\left(\langle\frac{W_\alpha^*-1}{\alpha}R_\varepsilon^{(*)}f, (H-\lambda+i\mu)R_\varepsilon f\rangle - \langle(H-\lambda+i\mu)R_\varepsilon^{(*)}f, \frac{W_\alpha^*-1}{\alpha}R_\varepsilon f\rangle\right)$$

or

$$\begin{aligned}\frac{dF_\varepsilon}{d\varepsilon} = \lim_{\alpha\to 0}\Bigg(&\langle R_\varepsilon^{(*)}f, \frac{W_\alpha - 1}{\alpha}f\rangle - \langle\frac{W_\alpha - 1}{\alpha}f, R_\varepsilon f\rangle \\ &+ \mathrm{i}\varepsilon\langle\frac{W_\alpha^*-1}{\alpha}R_\varepsilon^{(*)}f, H'R_\varepsilon f\rangle - \mathrm{i}\varepsilon\langle H'R_\varepsilon^{(*)}f, \frac{W_\alpha^*-1}{\alpha}R_\varepsilon f\rangle\Bigg)\end{aligned}$$

using

$$H''f = \lim_{\alpha\to 0}[\frac{W_\alpha^*-1}{\alpha}, H']f$$

we obtain the lemma. □

As an immediate consequence of these results, one gets the

Theorem B.16. *If J_ν is bounded or H'' is a bounded operator, there exists C' such that if* $\operatorname{dist}(I, J_\nu^c) > \eta > 0$ *then for all $\epsilon \in (0, \epsilon_0)$, for all $\lambda \in I$, for all $\mu \geq 0$, we have*

$$|F'_\varepsilon| \leq \frac{C'}{\sqrt{\varepsilon}}(|F_\varepsilon| + \|f\|^2_{D(A)})$$

for any $f \in D(A)$.

Proof – Let assume that H'' is bounded then we have

$$|F'_\varepsilon| \leq (\|R^*_\varepsilon f\|\|Af\| + \|Af\|\|R_\varepsilon f\| + \varepsilon\|H''\|\|R^*_\varepsilon f\|\|R_\varepsilon f\|$$

and so

$$|F'_\varepsilon| \leq \sqrt{C}(\frac{1}{\sqrt{\varepsilon}}\sqrt{|F_\varepsilon|}+\|f\|)\|Af\|+\sqrt{C}\|Af\|(\frac{1}{\sqrt{\varepsilon}}\sqrt{|F_\varepsilon|}+\|f|)+C\|H''\|\varepsilon(\frac{1}{\sqrt{\varepsilon}}\sqrt{|F_\varepsilon|}+\|f\|)^2$$

or

$$|F'_\varepsilon| \leq \sqrt{C}\frac{1}{\sqrt{\varepsilon}}(\sqrt{|F_\varepsilon|} + \|f\|)\|Af\| + \frac{1}{\sqrt{\varepsilon}}\|Af\|(\sqrt{|F_\varepsilon|} + \|f|) + C\|H''\|(\sqrt{|F_\varepsilon|} + \|f\|)^2$$

or if ε_0 is small enough

$$|F'_\varepsilon| \leq (C\|H''\| + 2\sqrt{C})\frac{1}{\sqrt{\varepsilon}}(|F_\varepsilon| + \|f\|^2_{D(A)}).$$

If J_ν is bounded then I is bounded and with $HR_\varepsilon = I - (\mathrm{i}\varepsilon H' - \lambda - \mathrm{i}\mu)R_\varepsilon$ we can adapt the proof. □

Then the Gronwall lemma gives

Theorem B.17 (Limiting absorption principle)**.** *There exist $\nu_0 > 0$ such that for $\eta > 0$, $\nu \leq \nu_0$ and $I \subset \mathbb{R}$ with* $\operatorname{dist}(I, J_\nu^c) > \eta$, *if J is bounded or $I \subset J \cap [-\frac{1}{\nu}, \frac{1}{\nu}]^c$ if J is unbounded in which case we also assume H'' is a bounded operator, such that the following holds. There exists $C > 0$ such that*

$$\sup_{\lambda \in I, \mu > 0} \langle f, (H - \lambda - \mathrm{i}\mu)^{-1} f\rangle.$$

Moreover the limits as $\mu \to \pm 0$ exits uniformly over I for the weak topology:

$$\lim_{\mu \to \pm 0} \langle f, (H - \lambda - \mathrm{i}\mu)^{-1} f\rangle$$

exits uniformly over I.

Proof – From the previous lemma on gets:

$$|F_\varepsilon - F_{\varepsilon_0}| \leq \int_\varepsilon^{\varepsilon_0} \frac{1}{\sqrt{\eta}}(|F_\eta| + \|f\|^2_{D(A)})\, d\eta$$

and so by Gronwall lemma:

$$|F_\varepsilon| \leq |F_{\varepsilon_0}| \exp(\sqrt{\varepsilon_0} - \sqrt{\varepsilon})$$

which gives the boundedness for $\varepsilon = 0$ since

$$|F_{\varepsilon_0}| \leq \|R_{\varepsilon_0} u\|\|u\| \leq \sqrt{\frac{C}{\varepsilon}}(\sqrt{|F_{\varepsilon_0}|} + \sqrt{\varepsilon}\|u\|)\|u\|$$

is bounded.

Then

$$|F_\varepsilon - F_{\varepsilon'}| \leq \int_\varepsilon^{\varepsilon'} \frac{1}{\sqrt{\eta}}(|F_\eta| + \|f\|^2_{D(A)})\, d\eta \leq \int_\varepsilon^{\varepsilon'} \frac{1}{\sqrt{\eta}}(|F_{\varepsilon_0}| \exp(\sqrt{\varepsilon_0} - \sqrt{\eta} + \|f\|^2_{D(A)})$$

which is hence a Cauchy sequence in $\varepsilon \to 0$. The resolvent identity and above estimates provides the uniform continuity of F_ε as $\mu \to 0$ and hence the theorem follows. □

Example B.18. *Consider $H = D_m$ in dimension $n = 3$ ($N = 4$) and $W_\alpha = e^{\mathrm{i}\alpha A}$ where A is the self-adjoint extension of*

$$\frac{1}{2}\left(D_m^{-1} P \cdot Q + Q \cdot P D_m^{-1}\right)$$

defined on smooth function with compact support. The domain of A contains

$$\left\{\psi \in L^2(\mathbb{R}^3)^4,\ x \mapsto x\psi(x) \in L^2(\mathbb{R}^3)^4\right\}$$

see [IM99]. Using [IM99, Identity (3.9)], [ABG96, Theorem 6.2.10] and the fact that smooth function with compact support form a core of A, we have

$$[iA, D_m] = \frac{-\Delta}{-\Delta + m^2}$$

implies that our assumptions are verified and H'' is bounded.

References

[ABG96] W. O. Amrein, A. Boutet de Monvel, and V. Georgescu. *C_0-groups, commutator methods and spectral theory of N-body Hamiltonians*. Vol. 135. Progress in Mathematics. Basel, 1996, pp. xiv+460.

[Amr+98] C. Amrouche, C. Bernardi, M. Dauge, and V. Girault. “ Vector potentials in three-dimensional non-smooth domains ”. In: *Math. Methods Appl. Sci.* 21.9 (1998), pp. 823–864.

[AY82] M. Arai and O. Yamada. “ Essential selfadjointness and invariance of the essential spectrum for Dirac operators ” . In: *Publ. Res. Inst. Math. Sci.* 18.3 (1982), pp. 973–985. DOI: 10.2977/prims/1195183289. URL: http://dx.doi.org/10.2977/prims/1195183289.

[BC12] N. Boussaïd and A. Comech. *On spectral stability of the nonlinear Dirac equation*. 2012. arXiv: 1211.3336 [math.AP].

[BM97] A. Boutet de Monvel and M. Măntoiu. *The method of the weakly conjugate operator*. Apagyi, Barnabás (ed.) et al., Inverse and algebraic quantum scattering theory. Proceedings of a conference, held at Lake Balaton, Hungary. 3–7 September 1996. Berlin: Springer. Lect. Notes Phys. 488, 204-226 (1997). 1997.

[BS90] M. Birman and M. Solomyak. “ The self-adjoint Maxwell operator in arbitrary domains ”. In: *Leningrad Math. J* 1.1 (1990), pp. 99–115.

[Che77] P. R. Chernoff. “ Schrödinger and Dirac operators with singular potentials and hyperbolic equations ”. In: *Pacific J. Math.* 72.2 (1977), pp. 361–382.

[Dir28] P. A. M. Dirac. “ The Quantum Theory of the Electron ” . In: *Royal Society of London Proceedings Series A* 117 (Feb. 1928), pp. 610–624. DOI: 10.1098/rspa.1928.0023.

[EL07] M. Esteban and M. Loss. “ Self-adjointness for Dirac operators via Hardy-Dirac inequalities ”. In: *J. Math. Phys.* 48.11 (2007), pp. 112107, 8.

[Gér08] C. Gérard. “ A proof of the abstract limiting absorption principle by energy estimates ” . In: *J. Funct. Anal.* 254.11 (2008), pp. 2707–2724. DOI: 10.1016/j.jfa.2008.02.015. URL: http://dx.doi.org/10.1016/j.jfa.2008.02.015.

[GGM04] V. Georgescu, C. Gérard, and J. S. Møller. “ Commutators, C_0-semigroups and resolvent estimates ”. In: *J. Funct. Anal.* 216.2 (2004), pp. 303–361.

[GJ07] S. Golénia and T. Jecko. “ A new look at Mourre's commutator theory. ” In: *Complex Anal. Oper. Theory* 1.3 (2007), pp. 399–422.

[GR86] V. Girault and P.-A. Raviart. *Finite element methods for Navier-Stokes equations*. Vol. 5. Springer Series in Computational Mathematics. Theory and algorithms. Berlin, 1986, pp. x+374.

[IM99] A. Iftimovici and M. Măntoiu. “ Limiting absorption principle at critical values for the Dirac operator ”. In: *Lett. Math. Phys.* 49.3 (1999), pp. 235–243.

[Kal98] H. Kalf. “ Essential self-adjointness of Dirac operators under an integral condition on the potential ” . In: *Lett. Math. Phys.* 44.3 (1998), pp. 225–232. DOI: 10.1023/A:1007415716921. URL: http://dx.doi.org/10.1023/A:1007415716921.

[Kat66] T. Kato. “ Wave operators and similarity for some non-selfadjoint operators ”. In: *Math. Ann.* 162 (1965/1966), pp. 258–279.

[Kes61] H. Kestelman. “ Anticommuting linear transformations ”. In: *Canad. J. Math.* 13 (1961), pp. 614–624.

[Kla80] M. Klaus. “ Dirac operators with several Coulomb singularities ”. In: *Helv. Phys. Acta* 53.3 (1980), 463–482 (1981).

[KY01] H. Kalf and O. Yamada. “ Essential self-adjointness of n-dimensional Dirac operators with a variable mass term ” . In: *J. Math. Phys.* 42.6 (2001), pp. 2667–2676. DOI: 10.1063/1.1367331. URL: http://dx.doi.org/10.1063/1.1367331.

[KY89] T. Kato and K. Yajima. “ Some examples of smooth operators and the associated smoothing effect ” . In: *Rev. Math. Phys.* 1.4 (1989), pp. 481–496. DOI: 10.1142/S0129055X89000171. URL: http://dx.doi.org/10.1142/S0129055X89000171.

[LO77] B. M. Levitan and M. Otelbaev. “ Conditions for the selfadjointness of Schrödinger and Dirac operators ”. In: *Dokl. Akad. Nauk SSSR* 235.4 (1977), pp. 768–771.

[LR79] J. J. Landgren and P. A. Rejto. “ An application of the maximum principle to the study of essential selfadjointness of Dirac operators. I ” . In: *J. Math. Phys.* 20.11 (1979), pp. 2204–2211. DOI: 10.1063/1.523999. URL: http://dx.doi.org/10.1063/1.523999.

[LRK80] J. J. Landgren, P. A. Rejto, and M. Klaus. " An application of the maximum principle to the study of essential selfadjointness of Dirac operators. II " . In: *J. Math. Phys.* 21.5 (1980), pp. 1210–1217. DOI: 10.1063/1.524546. URL: http://dx.doi.org/10.1063/1.524546.

[Mou81] E. Mourre. " Absence of singular continuous spectrum for certain selfadjoint operators ". In: *Comm. Math. Phys.* 78.3 (1980/81), pp. 391–408. URL: http://projecteuclid.org/euclid.cmp/1103908694.

[Nen75] G. Nenciu. " Eigenfunction expansions for Schrödinger and Dirac operators with singular potentials ". In: *Comm. Math. Phys.* 42 (1975), pp. 221–229.

[Pau36] W. Pauli. " Contributions mathématiques à la théorie des matrices de Dirac ". In: *Ann. Inst. H. Poincaré* 6.2 (1936), pp. 109–136. URL: http://www.numdam.org/item?id=AIHP_1936__6_2_109_0.

[Put67] C. R. Putnam. *Commutation properties of Hilbert space operators and related topics*. Ergebnisse der Mathematik und ihrer Grenzgebiete, Band 36. 1967, pp. xi+167.

[Ran] A. F. Ranada. "Classical nonlinear Dirac field models of extended particles". In: *Quantum theory, groups, fields and particles,* vol. 198. Amsterdam, Reidel, pp. 271–291.

[RS04] I. Rodnianski and W. Schlag. " Time decay for solutions of Schrödinger equations with rough and time-dependent potentials " . In: *Invent. Math.* 155.3 (2004), pp. 451–513. DOI: 10.1007/s00222-003-0325-4. URL: http://dx.doi.org/10.1007/s00222-003-0325-4.

[RS78] M. Reed and B. Simon. *Methods of modern mathematical physics. IV. Analysis of operators*. New York, 1978, pp. xv+396.

[RS79] M. Reed and B. Simon. *Methods of modern mathematical physics. III.* Scattering theory. 1979, pp. xv+463.

[RS80] M. Reed and B. Simon. *Methods of modern mathematical physics. I.* Second. Functional analysis. New York, 1980, pp. xv+400.

[Shi11] D. S. Shirokov. " Extension of Pauli's theorem to the case of Clifford algebras " . In: *Dokl. Akad. Nauk* 440.5 (2011), pp. 607–610. DOI: 10.1134/S1064562411060329. URL: http://dx.doi.org/10.1134/S1064562411060329.

[Shi13] D. Shirokov. " Pauli theorem in the description of n-dimensional spinors in the Clifford algebra formalism " . In: *Theoretical and Mathematical Physics* 175.1 (2013), pp. 454–474. DOI: 10.1007/s11232-013-0038-9. URL: http://dx.doi.org/10.1007/s11232-013-0038-9.

[Tha92] B. Thaller. *The Dirac equation*. Texts and Monographs in Physics. Berlin, 1992, pp. xviii+357. DOI: 10.1007/978-3-662-02753-0. URL: http://dx.doi.org/10.1007/978-3-662-02753-0.

[Wae74] B. L. van der Waerden. *Group theory and quantum mechanics*. Translated from the 1932 German original, Die Grundlehren der mathematischen Wissenschaften, Band 214. New York, 1974, pp. viii+211.

[Xia99] J. Xia. " On the contribution of the Coulomb singularity of arbitrary charge to the Dirac Hamiltonian " . In: *Trans. Amer. Math. Soc.* 351.5 (1999), pp. 1989–2023. DOI: 10.1090/S0002-9947-99-02084-X. URL: http://dx.doi.org/10.1090/S0002-9947-99-02084-X.

Part II

The PhD Thesis

II.3

Description of the PhD thesis

For the reader convenience, we present here the results we obtained during the PhD, see [Bou06a] and [Bou06b; Bou08; Bou07].

My PhD thesis was devoted to the study of the stability of small stationary solutions of a non-linear Dirac equation :

$$\mathrm{i}\partial_t \psi = (D_m + V)\,\psi + \nabla F(\psi).$$

where $F \in C^\infty(\mathbb{C}^4, \mathbb{R})$ was such that

$$F(e^{\mathrm{i}\theta} z) = F(z),\ \forall \theta \in \mathbb{R},\ \forall z \in \mathbb{C}^4.$$

and $V \in C^\infty(R^3, \mathcal{S}_4(\mathbb{C}))$, where $S_4(\mathbb{C})$ is the space of self-adjoint 4×4 matrices, was such that there exists $\rho > 5$ with

$$\forall \alpha \in \mathbb{N}^3,\ \exists C > 0,\ \forall x \in \mathbb{R}^3,\ |\partial^\alpha V|(x) \leq \frac{C}{\langle x \rangle^{\rho+|\alpha|}}.$$

We considered stationary state $e^{-\mathrm{i}tE}\psi_0$ where $E \in \mathbb{R}$ and

$$E\psi_0 = (D_m + V)\,\psi_0 + \nabla F(\psi_0).$$

In these analysis, the non-linear equations were viewed as small non-linear perturbations of linear systems. A part of the PhD thesis was hence devoted to the study of linear problems. We proved that for the Dirac operator $H := D_m + V$ with no resonance at thresholds nor eigenvalue at thresholds, the propagator satisfies propagation and dispersive estimates. We also deduced Kato smoothness estimates and Strichartz estimates.

With some *ad hoc* assumptions on the discrete spectrum of a Dirac operator, we built small manifolds of stationary states. Then with small variations on these assumptions, we highlighted some stabilization process and orbital instability phenomena for some stationary states.

3.1 The linear theory

Below $\mathbf{P}_c(H) = \mathbb{1}_{(-\infty,-m]\cup[+m,+\infty)}(H)$ is the projector associated with the continuous spectrum of H and $\mathcal{H}_c = \mathbf{P}_c(H)L^2(\mathbb{R}^3, \mathbb{C}^4)$.

We needed precise decay estimates of e^{-itH} in $\mathcal{H}_c$ in order to analyse the stabilisation properties of the non-linear system.

For this, we made the

Assumption 3.1.1. *The operator H presents no resonance at thresholds and no eigenvalue at thresholds.*

A resonance is a solution of

$$E\phi = (D_m + V)\phi$$

in $H^{1/2}_{-\sigma}(\mathbb{R}^3, \mathbb{C}^4) \setminus H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ for some $\sigma \in (1/2, \rho - 1/2)$.

3.1.1 The propagation estimates

We obtained the

Theorem 3.1 (Propagation for perturbed Dirac dynamics)**.** *Let $\sigma > 5/2$. Then one has*

$$\|e^{-\mathrm{i}tH}\mathbf{P}_c(H)\|_{B(L^2_\sigma, L^2_{-\sigma})} \le C\langle t\rangle^{-3/2}.$$

Where $\|f\|_{L^2_\sigma} = \|\langle Q\rangle^\sigma f\|_{L^2}$.

The proof was divided in two parts :

1. High and intermediate energies were treated by means of a minimal escape velocity (based on Mourre estimates, see Appendix B);
2. Thresholds (or low) energies used ideas from [JK79] and hence asymptotic expansion of resolvent at thresholds where we used Assumption 3.1.1.

Using Bochner-Fourier transform, we deduce the a consequence of this result is the

Theorem 3.2 (H-smoothness of $\langle Q\rangle^{-1}$)**.** *We have for any $s \in \mathbb{R}$*

$$\int_{\mathbb{R}} \|\langle Q\rangle^{-1} e^{-\mathrm{i}tH}\mathbf{P}_c(H)\psi\|^2_{H^s}\, dt \le C\|\psi\|^2_{H^s},$$

$$\|\int_{\mathbb{R}} e^{\mathrm{i}tH}\mathbf{P}_c(H)\langle Q\rangle^{-1}F(t)\,dt\|_{H^s} \le C\|F\|_{L^2(\mathbb{R},H^s)},$$

$$\|\int_{s<t}\langle Q\rangle^{-1} e^{-\mathrm{i}(t-s)H}\mathbf{P}_c(H)\langle Q\rangle^{-1}F(s)\,ds\|_{L^2(\mathbb{R},H^s)} \le C\|F\|_{L^2_t(\mathbb{R},H^s)},$$

3.1.2 The dispersive estimates

In the forthcoming sections, our results are based in an *a priori* analysis of a Cauchy problem. To close these *a priori* estimates we need the above propagation properties. Unfortunately they were not sufficient, we also proved the

Theorem 3.3 (Dispersive estimates)**.** *For any $\theta \in [0,1]$, $p \in [1,2]$, $s - s' \ge (2+\theta)(\frac{2}{p} - 1)$ and $p' = p/(p-1)$, there exists $C > 0$ such that*

$$\|e^{-\mathrm{i}tH}\mathbf{P}_c(H)\|_{B^s_{p,q}, B^{s'}_{p',q}} \le C \begin{cases} |t|^{(-1+\theta/2)(\frac{2}{p}-1)} & \textit{if } |t| \in (0,1] \\ |t|^{(-1-\theta/2)(\frac{2}{p}-1)} & \textit{if } |t| \in [1,\infty) \end{cases}.$$

The method of proof in the free case ($V = 0$) is classical in the sense that is based on oscillatory integrals estimates using the dispersion relations of the system. These integrals appear via a Fourier transform which in a sense diagonalises the free Dirac operator. It was tempting to mimic the procedure in the general case by using a kind of distorted Fourier transform based on distorted plane waves or expansions with respect to the generalised eigenvectors.

By means of the TT^* method or actually using the result by [KT98], this in turn implied the

Theorem 3.4 (Strichartz-type estimates). *For any* $2 \leq p, q \leq \infty$, $\theta \in [0,1]$, *for* $\beta \in [-\theta/2, \theta/2]$ *such that* $(1-\frac{2}{q})(1+\beta) = \frac{2}{p}$ *with* $(p,\beta) \neq (2,0)$, *taking* $\alpha(q) = (1+\frac{\theta}{2})(1-\frac{2}{q})$ *and* $s' - s \geq \alpha(q)$, *there is a positive constant* C *such that*

$$\|e^{-\mathrm{i}tH} P_c(H)\psi\|_{L^p_t(\mathbb{R}, B^s_{q,2}(\mathbb{R}^3,\mathbb{C}^4))} \leq C\|\psi\|_{H^{s'}(\mathbb{R}^3,\mathbb{C}^4)},$$
$$\|\int e^{\mathrm{i}tH} P_c(H)F(t)\,dt\|_{H^s} \leq C\|F\|_{L^{p'}(\mathbb{R}, B^{s'}_{q',2}(\mathbb{R}^3,\mathbb{C}^4))},$$
$$\|\int_{s<t} e^{-\mathrm{i}(t-s)H} P_c(H)F(s)\,ds\|_{L^p(\mathbb{R}, B^{-s}_{q,2}(\mathbb{R}^3,\mathbb{C}^4))} \leq C\|F\|_{L^{\tilde{p}'}(\mathbb{R}, B^{\tilde{s}}_{\tilde{q}',2}(\mathbb{R}^3,\mathbb{C}^4))},$$

for any $r \in [1,\infty]$ *and* $(\tilde{q},\tilde{p})$ *chosen like* (q,p) *and* $s + \tilde{s} \geq \alpha(q) + \alpha(\tilde{q})$.

3.2 The one eigenvalue case

In the simplest case [Bou07], we assumed that the operator $H := D_m + V$ has only *one simple eigenvalue* λ_0 and denote by ϕ_0 an associated normalised eigenvector.

3.2.1 The PLS manifold

Out of this assumption, stationary solutions are built by bifurcation methods. We have the

Proposition 3.5. *For any* $\sigma \in \mathbb{R}^+$, *there exists a neighbourhood* Ω *of* $0 \in \mathbb{C}$, *a* C^∞ *map*

$$h : \Omega \mapsto \mathcal{H}_c \cap H^2(\mathbb{R}^3,\mathbb{C}^4) \cap L^2_\sigma(\mathbb{R}^3,\mathbb{C}^4)$$

and a C^∞ *map* $E : \Omega \mapsto \mathbb{R}$ *such that*

$$\boxed{S(U) = U\phi_0 + h(U)}$$

satisfies for all $U \in \Omega$,

$$HS(U) + \nabla F(S(U)) = E(U)S(U),$$

with the following properties

$$\begin{array}{rcl} h(e^{\mathrm{i}\theta}U) &=& e^{\mathrm{i}\theta}h(U),\ \forall\theta \in \mathbb{R} \\ \|h(U)\|_{H^2\cap L^2_\sigma} &=& O(|U|^2) \\ E(U) &=& E(|U|)\ = \lambda_0 + O(|U|^2). \end{array}$$

By means of classical methods, we inferred the

Lemma 3.6. *For any* $\alpha \in \mathbb{N}^2$, $s \in \mathbb{R}^+$ *and* $p, q \in [1,\infty]$ *there is* $\gamma > 0$, $\varepsilon > 0$ *and* $C > 0$ *such that for all* $U \in B_{\mathbb{C}^2}(0,\varepsilon)$ *one has*

$$\|e^{\gamma\langle Q\rangle}\partial^\alpha_U S(U)\|_{B^s_{p,q}} \leq C\|S(U)\|_2.$$

The space $B^s_{p,q}$ is the usual Besov space on $\mathbb{R}^3$.

3.2.2 The stability problem

For a perturbation

$$\psi_0 = S(U_0) + \eta_0,$$

the associated solution can be written

$$\psi(t) = e^{-\mathrm{i}\int_0^t E(U(s))\,ds}\left[S(U(t)) + \eta(t)\right].$$

We wanted toe track the evolution of U and η. In order to write a modulation equation for U and an equation for η, we imposed $\eta \in \mathcal{H}_0^\perp(U)$ where

$$\mathcal{H}_0^\perp(U) = \left\{\eta \in L^2(\mathbb{R}^3, \mathbb{C}^8), \left\langle J\eta, \frac{\partial}{\partial \Re U} S(U)\right\rangle = \left\langle J\eta, \frac{\partial}{\partial \Im U} S(U)\right\rangle = 0\right\},$$

which is invariant under the action of $JH(U)$. The skew-adjoint operator J represents the action of $-\mathrm{i}$ on $\mathbb{C}$ when the later is identified with $\mathbb{R}^2$.

So we wanted to solve the equation

$$\begin{aligned}\partial_t \eta &= J\{H - E(U)\}\eta + J\{\nabla F(S(U)+\eta) - \nabla F(S(U))\} + dS(U)\dot{U}\\ &= J\{H + d^2F(S(U)) - E(U)\}\eta + JN(U,\eta) + dS(U)\dot{U}\end{aligned}$$

for $\eta \in \mathcal{H}_0^\perp(U(t))$. The notation $d^2F(S(U))$ stand for the differential of the gradient of F, which is no longer $\mathbb{C}$-linear as the differential with respect to the real structure. Below we write $H(U)$ for $H + d^2F(S(U)) - E(U)$.

The condition

$$\langle \eta(t), JdS(U(t))\rangle = 0,$$

after a time derivation gives:

$$\dot{U}(t) = -A(U(t), \eta(t))\langle N(U(t), \eta(t)), dS(U(t))\rangle$$

where A is a smooth non vanishing function.

We obtained the following equation

$$\partial_t \eta = J\left\{H + d^2F(S(U)) - E(U)\right\}\eta + J\widetilde{N}(U,\eta)$$

where

$$|\widetilde{N}(U,\eta)| \le C(U,\eta)|\eta|^2$$

where C is locally bounded in U and η.

Notice that the function η is $\mathbb{C}^8$-valued. This is due to a two steps process. First, $\mathbb{C}$ is replaced by $\mathbb{R}^2$ as the linear part of the equation is not $\mathbb{C}$ but $\mathbb{R}$ linear, and then the operator and the function are complexified.

The idea was then to solve this equation in a space of functions which tend to 0 asymptotically in time. Somehow we wanted to consider the wellposedness of this equation in some well chosen functional setting.

In order to analyse the wellposedness, we needed some dispersive properties on the linear part. Due to the smallness assumption on the initial state, the estimates for H were enough.

3.2.3 Stabilisation and non-linear scattering

The functional setting we considered is given by the set:

$$S = \left\{ (U, \eta) \,;\; U \in \Omega,\; \eta \in \mathcal{H}_c(U) \cap H^s(\mathbb{R}^3, \mathbb{C}^4) \right\},$$

endowed with the norm of $\mathbb{C}^2 \times H^s$ for some $s > 2$. Here $\mathcal{H}_c(U) := \mathcal{H}_0^\perp(U)$ but later it will change.

Hence by solving a fixed point problem, we obtained the stability trough the

Theorem 3.7 (Stabilisation)**.** *Let $s > \beta + 2 > 2$ and $\sigma > 3/2$, there exist $\mathcal{V}_0$ a neighbourhood of $(0,0)$ in S and $C > 0$ such that for any initial condition of the form $\psi_0 = S(U_0) + \eta_0$ with $(U_0, \eta_0) \in \mathcal{V}_0$, one has*

(i) there exists a unique global solution ψ and this solution is in $C(\mathbb{R}, H^s) \cap \mathcal{C}(\mathbb{R}, H^{s-1})$;

(ii) there exist $U_{\pm\infty}$, with

$$|U_{\pm\infty} - U_0| \leq C \|\eta_0\|^2_{H^s},$$

such that for all $t \in \mathbb{R}$

$$\psi(t) = e^{-\mathrm{i} \int_0^t E(U(v))\, dv} S(U(t)) + \varepsilon_\pm(t)$$

with $\dot U \in L^p(\mathbb{R})$ for all $p \in [1, \infty]$, $\lim\limits_{t \to \pm\infty} U(t) = U_{\pm\infty}$ and

$$\max \left\{ \|\varepsilon_\pm\|_{L^\infty(\mathbb{R}^\pm, H^s)} ,\; \|\varepsilon_\pm\|_{L^2(\mathbb{R}^\pm, H^s_{-\sigma})} ,\; \|\varepsilon_\pm\|_{L^2(\mathbb{R}^\pm, B^\beta_{\infty,2})} \right\} \leq C \|\eta_0\|_{H^s}.$$

The above theorem can be rephrased as : any small solution relaxes towards the manifold of stationary solutions.

One can notice that the asymptotic of the phase is rather unclear. To clarify this point the above theorem can be refined using pointwise decay estimates (Theorems 3.1 and 3.3 instead of Theorems 3.2 and 3.4) and thus imposing localisation on the perturbation. As a by-product we can also refine the asymptotic of the other terms.

Thus considering the set

$$\mathcal{S}_\sigma = \left\{ (U, z) \,;\; U \in B_{\mathbb{C}^2}(0, \varepsilon),\; z \in \mathcal{H}_c(U) \cap B_{H^s_\sigma}(0, r(U)) \right\}$$

endowed with the metric $\mathbb{C}^2 \times H^s_\sigma$, we obtained the

Theorem 3.8 (Nonlinear scattering)**.** *Let $s > \beta + 3 > 6$ and $\sigma > 5/2$, there exist $\mathcal{V}_\sigma$ a neighbourhood of $(0,0)$ in S_σ and $C > 0$ such that for any initial condition of the form $\psi_0 = S(U_0) + \eta_0$ with $(U_0, \eta_0) \in S_\sigma$, there exist bijective maps $(V_{\pm\infty}; \eta_\pm) : \mathcal{V}_0 \mapsto \mathcal{V}^\pm_\sigma$, where $\mathcal{V}^\pm_\sigma$ are open neighbourhoods of $(0,0)$ in S_σ with*

$$|V_{\pm\infty} - U_0| \leq C \|\eta_0\|^2_{H^s}, \|\eta_\pm - \eta_0\|_{H^s} \leq C \|\eta_0\|^2_{H^s},$$

such that for all $t \in \mathbb{R}$

$$\psi(t) = e^{-\mathrm{i} t E(V_{\pm\infty})} S(V_\pm(t)) + e^{-\mathrm{i} t E(V_{\pm\infty})} e^{-\mathrm{i} t H(V_{\pm\infty})} \eta_\pm + \varepsilon_\pm(t)$$

with $\dot V_\pm + \mathrm{i}\,(E(V_\pm) - V_{\pm\infty}) \in L^p(\mathbb{R})$ for all $p \in [1, \infty]$, $\lim\limits_{t \to \pm\infty} V_\pm(t) = V_{\pm\infty}$ and

$$\begin{aligned}
\left| \dot V_\pm(t) + \mathrm{i}\,(E(V_\pm(t)) - E(V_{\pm\infty})) \right| &\leq \frac{C}{\langle t \rangle^2} \|z_0\|^2_{H^s_\sigma}, \\
|V_\pm(t) - V_{\pm\infty}| &\leq \frac{C}{\langle t \rangle} \|z_0\|_{H^s_\sigma}, \\
\max \left\{ \|\varepsilon_\pm(t)\|_{H^s} ,\; \|\varepsilon_\pm(t)\|_{H^s_{-\sigma}} , \|\varepsilon_\pm(t)\|_{B^\beta_{\infty,2}} \right\} &\leq \frac{C}{\langle t \rangle^2} \|z_0\|^2_{H^s_\sigma} \\
\text{and } \left\| e^{-J t H(V_{\pm\infty})} e^{J \int_0^t (E(V_\pm(s)) - E(V_{\pm\infty})\, ds} \varepsilon_\pm(t) \right\|_{H^s_{\frac{3}{2}}} &\leq \frac{C}{\langle t \rangle^{\frac{1}{2}}} \|z_0\|^2_{H^s_\sigma}.
\end{aligned}$$

Moreover, the maps $(U_0; z_0) \in \mathcal{V}_\sigma \mapsto (U_{\pm\infty}; z_{\pm\infty}) \in \mathcal{V}_\sigma^\pm$ *are bijective.*

3.3 The two eigenvalues case

3.3.1 The two eigenvalues case with non resonant condition

In [Bou06b], the operator H has two simple eigenvalue λ_0 and λ_1 in a non resonant configuration for the first one:

$$|\lambda_1 - \lambda_0| < \min\{|\lambda_0 + m|, |\lambda_0 - m|\}.$$

This assumption was useful in our study of the spectrum of the linearised operator around a stationary state, it gave us that this operator has two simple non zero eigenvalues.

3.3.1.1 PLS manifold

We proved in Theorem 3.9 that some solutions are global and can be decomposed as the sum of a stationary solution plus a remainder part which is vanishing. Since the stationary solution part may change during the evolution, we need to track it. Again we built, as in Proposition 3.5, with bifurcation methods, a map $S : \Omega \subset \mathbb{C} \mapsto H^2(\mathbb{R}^3, \mathbb{C}^4) \cap L^2_\sigma(\mathbb{R}^3, \mathbb{C}^4)$ and $E : \Omega \mapsto \mathbb{R}$ such that

$$E(u)S(u) = HS(u) + \nabla F(S(u)).$$

We also obtained the exponential decay of Lemma 3.6.

3.3.1.2 Stable manifold

The linearised operator $JH(U)$ around a stationary state $S(U)$ has a two dimensional geometric kernel and two simple eigenvalues $E_1(U)$ and $-E_1(U)$ which are purely imaginary. The associated eigenspaces are conjugated one to each other. Working on the real part of their direct sum, we introduced a family of basis of this last real space : $(\phi_1^1(U), \phi_1^2(U))$.

The rest of the spectrum is the essential spectrum. We write $\mathcal{H}_c(U)$ for the space associated with the continuous spectrum. This space $\mathcal{H}_c(U)$ is the orthogonal of the previous eigenspaces with respect to the product $(f, g) \mapsto \Re\langle f, Jg\rangle$ where $\langle\cdot,\cdot\rangle$ is the standard product of $L^2(\mathbb{R}^3, \mathbb{C}^4)$.

Since there is a second eigenvalue, we obtained only stable directions with the

Theorem 3.9 (Stable manifold)**.** *Let* $s, s', \beta \in \mathbb{R}_+^*$ *be such that* $s' \geq s + 3 \geq \beta + 6$ *and* $\sigma > 5/2$*. There exist* $\varepsilon_0 > 0$*,* $R > 0$*,* $K > 0$*,* $T_0 > 0$ *and Lipschitz map*

$$\Psi : \mathcal{S} \mapsto \mathbb{R}^2$$

where $\mathcal{S} = \left\{(V, \xi)\,;\; V \in B_{\mathbb{C}^2}(0, \varepsilon),\; \xi \in \mathcal{H}_c(U) \cap B_{H^{s'}_\sigma}(0, R)\right\}$ *endowed with the metric of* $\mathbb{C}^2 \times H^{s'}_\sigma$ *with* $\Psi(U, 0) = 0$ *for all* $U \in B_{\mathbb{C}}(0, \varepsilon)$*,*

$$|\Psi(U, z)| \leq K\left(|U| + \|z\|_{H^{s'}_\sigma}\right)^2,$$

such that the following holds. For any initial condition of the form

$$\psi_0 = S(U_0) + z_0 + \Psi(U_0, z_0) \cdot \phi_1(U_0)$$

with $(U_0, z_0) \in \mathcal{S}$*, one has* *(i) there exists a unique solution ψ with initial condition ψ_0, and this solution is in*

$$\mathcal{C}\left((-T_0;+\infty), H^{s'}(\mathbb{R}^3,\mathbb{C}^4)\right) \cap \mathcal{C}^1\left(]-T_0;+\infty[, H^{s'-1}(\mathbb{R}^3,\mathbb{C}^4)\right);$$

(ii) there exist $(U_\infty, z_\infty) \in \mathcal{S}$ and $E_\infty \in \mathbb{R}$ with

$$|U_\infty - U_0| \leq K\|z_0\|^2_{H^{s'}_\sigma}, \quad |E_\infty| \leq K\|z_0\|^2_{H^{s'}_\sigma}, \quad \|z_\infty - z_0\|_{H^{s'}} \leq K\|z_0\|^2_{H^{s'}_\sigma}$$

such that

$$\psi(t) = e^{-\mathrm{i}(tE(U_\infty)+E_\infty+r(t))}\left(S(U_\infty) + e^{JtH(U_\infty)}z_\infty + \varepsilon(t)\right),$$

where

$$\begin{cases} \|\varepsilon(t)\|_{H^{s'}} \leq \dfrac{K}{\langle t\rangle}\|z_0\|^2_{H^{s'}_\sigma} \\ \|\varepsilon(t)\|_{H^{s}_{-\sigma}} \leq \dfrac{K}{\langle t\rangle^2}\|z_0\|^2_{H^{s'}_\sigma} \\ \|\varepsilon(t)\|_{B^{\beta}_{\infty,2}} \leq \dfrac{K}{\langle t\rangle^2}\|z_0\|^2_{H^{s'}_\sigma} \end{cases}$$

and $|r(t)| \leq \frac{K}{\langle t\rangle}\|z_0\|^2_{H^{s'}_\sigma}$ as $t \to +\infty$.

A version of this theorem with no localisation in the perturbation (similarly to Theorem 3.7) could be obtained by using Theorems 3.2 and 3.4.

3.3.2 The two eigenvalues case with a non resonant condition

In [Bou08] H has two simple eigenvalues λ_0 and λ_1. We denote some associated normalised eigenvectors by ϕ_0 and ϕ_1 a resonant condition for the first one

$$|\lambda_1 - \lambda_0| > \min\{|\lambda_0 + m|, |\lambda_0 - m|\}. \tag{3.1}$$

There again we obtained a smooth map

$$S : \Omega \subset \mathbb{C} \mapsto H^2(\mathbb{R}^3,\mathbb{C}^4) \cap L^2_\sigma(\mathbb{R}^3,\mathbb{C}^4)$$

and a C^∞ map $E : \Omega \mapsto \mathbb{R}$ such that

$$HS(U) + \nabla F(S(U)) = E(U)S(U)$$

with the exponential decay.

The resonant condition we imposed is the Fermi Golden Rule

$$\Gamma(\phi_0) := \lim_{\substack{\varepsilon\to 0,\\ \varepsilon>0}} \left\langle d^2F(\phi_0)\phi_1, \Im\left((H-\lambda_0) + (\lambda_1-\lambda_0) - \mathrm{i}\varepsilon\right)^{-1} P_c(H) d^2F(\phi_0)\phi_1\right\rangle > 0. \tag{3.2}$$

The quantity $\Gamma(\phi_0)$ is always non-negative, the assumption is thus that it is non-zero. This kind of assumption is considered as generic with respect to F.

Due to condition 3.1 and 3.2, we were able to give a more exhaustive description of the non-linear flow in the vicinity of a small stationary solution $S(U)$.

3.3.2.1 The stabilisation

This time beside the kernel there is four eigenvalues $\pm E_1(U)$ and $\pm\overline{E_1}(U)$ with non zero real parts due to the resonant condition and the Fermi golden rule. There is no other points in the point spectrum. For the associated sum of eigenspaces $\mathcal{H}^1_+(U)$, we introduced a basis $(\xi_i(U))_{i=1,\dots,4}$ of $\mathcal{H}^1_+(U)$. The space $\mathcal{H}_c(U)$ has the same definition and we introduced

$$S = \{(U,z)\,;\; U \in B_{\mathbb{C}}(0,\varepsilon),\; z \in \mathcal{H}_c(U) \cap B_{H^s}(0, r(U))\}$$

endowed with the metric of $\mathbb{C} \times H^s$.

We obtained again stable directions in the

Theorem 3.10. *For $s > \beta + 2 > 2$ and $\sigma > 3/2$, there exist $\varepsilon > 0$, $C > 0$, a continuous map $r : B_{\mathbb{C}}(0,\varepsilon) \mapsto \mathbb{R}$ with $r(U) = O(|U|^2)$, $\mathcal{V}$ a neighbourhood $(0,0)$ in S and a map $\Psi : \mathcal{V} \mapsto \mathbb{R}^8$, smooth n $\mathcal{V} \setminus (0,0)$ with for $U \in B_{\mathbb{C}^2}(0,\varepsilon)$*

$$\|\Psi(U,z)\| = O(\|z\|^2_{H^s})$$

for all $z \in \mathcal{H}_c(U) \cap B_{H^s}(0, r(U))$ with $(U,z) \in \mathcal{V}$ such that the following holds.

For any initial condition of the form $\psi_0 = S(U_0) + z_0 + A \cdot \xi(U_0)$ with $(U_0, z_0) \in \mathcal{V}$ and $A = \Psi(U_0, z_0)$,

(i) there exists a unique global solution ψ and this solution is in $C(\mathbb{R}, H^s) \cap C(\mathbb{R}, H^{s-1})$;

(ii) there exist $U_{\pm\infty}$, with $|U_{\pm\infty} - U_0| \le C\|z_0\|^2_{H^s}$, such that for all $t \in \mathbb{R}$

$$\psi(t) = e^{-\mathrm{i}\int_0^t E(U(v))\,dv} S(U(t)) + \varepsilon_\pm(t)$$

with $\dot{U} \in L^p(\mathbb{R})$ for all $p \in [1,\infty]$, $\lim_{t\to\pm\infty} U(t) = U_\pm$ and

$$\max\left\{ \|\varepsilon_\pm\|_{L^\infty(\mathbb{R}^\pm, H^s)},\ \|\varepsilon_\pm\|_{L^2(\mathbb{R}^\pm, H^s_{-\sigma})},\ \|\varepsilon_\pm\|_{L^2(\mathbb{R}^\pm, B^\beta_{\infty,2})} \right\} \le C\|z_0\|_{H^s}.$$

The set

$$\mathcal{CM} := \{S(U_0) + z_0 + A \cdot \xi(U_0),\ \text{with } (U_0, z_0) \in \mathcal{V} \text{ and } A = \Psi(U_0, z_0)\}$$

plays the role of the central manifold as it is build with components that are associated with the central spectrum, that is part of the spectrum of the linearised operator with zero real part.

3.3.2.2 Stable and unstable directions

We introduce the set

$$\widetilde{S} = \{(U,z,p)\,;\; U \in B_{\mathbb{C}}(0,\varepsilon),\; z \in \mathcal{H}_c(U) \cap B_{H^s}(0, r(U)), p \in B_{\mathbb{R}^4}(0, r(U)),\}$$

endowed with the metric of $\mathbb{C} \times H^s \times \mathbb{R}^4$.

Using the resonant condition, we were able to treat the transverse directions to the stable manifold in the

Theorem 3.11. *For $s > 2$, there exist $C > 0$, $\mathcal{W}_\pm$ neighbourhoods of $(0,0,0)$ in $\widetilde{S}$ and maps $\Phi_\pm : \mathcal{W}_\pm \mapsto \mathbb{R}^8$, smooth on $\mathcal{W}_\pm \setminus \{(0,0,0)\}$ with*

$$\|\Phi_\pm(U,z,p)\| = O(\|z\|^2_{H^s} + \|p\|^2_{H^s}), \quad \forall (U,z,p) \in \mathcal{W}_\pm$$

and such that for any initial condition of the form

$$\psi_0 = S(U_0) + z_0 + (p_+, p_-).\xi(U_0, z_0)$$

which is not in $\mathcal{CM}$, the following holds.

- *If* $(U_0, z_0, p_+) \in \mathcal{W}_+$ *and* $p_- = \Phi_+(U_0, z_0, p_+)$ *then for any small neighbourhood* $\mathcal{O}$ *of* $S(U_0)$ *including* ψ_0 *there exists* $t_+(\psi_0) > 0$ *and a unique solution* $\psi \in \cap_{k=0}^2 C^k([-t_+; +\infty), H^{s-k})$ *with* $\psi(0) = \psi_0$.

  Moreover we have

$$\mathrm{dist}(\psi(t), \mathcal{CM})_{H^s} \leq C\mathrm{dist}(\psi_0, \mathcal{CM})_{H^s} e^{-\gamma t} \text{ when } t \to +\infty \quad \text{and} \quad \psi_+(-t_+) \notin \mathcal{O}$$

  where γ *is in a ball of centre* $1/2\Gamma(U_0)$ *and radius* $O(|U_0|^6))$.

- *If* $(U_0, z_0, p_-) \in \mathcal{W}_-$ *and* $p_+ = \Phi_-(U_0, z_0, p_-)$ *then for any small neighbourhood* $\mathcal{O}$ *of* $S(U_0)$ *including* ψ_0 *there exists* $t_-(\psi_0) > 0$ *and a unique solution* $\psi \in \cap_{k=0}^2 C^k((-\infty; t_-), H^{s-k})$ *with* $\psi(0) = \psi_0$.

  Moreover we have

$$\mathrm{dist}(\psi(t), \mathcal{CM})_{H^s} \leq C\mathrm{dist}(\psi_0, \mathcal{CM})_{H^s} e^{\gamma t} \text{ when } t \to -\infty \quad \text{and} \quad \psi_-(t_-) \notin \mathcal{O}$$

  where γ *is in a ball of centre* $1/2\Gamma(U_0)$ *and radius* $O(|U_0|^6))$.

3.3.2.3 The non-linear scattering

Consider the set

$$\mathcal{S}_\sigma = \left\{(U, z)\,;\ U \in B_{\mathbb{C}^2}(0, \varepsilon),\ z \in \mathcal{H}_c(U) \cap B_{H^s_\sigma}(0, r(U))\right\}$$

endowed with the metric $\mathbb{C}^2 \times H^s_\sigma$.

We also proved a scattering result, using Theorems 3.2 and 3.3, in the

Theorem 3.12. *For* $s > \beta + 2 > 2$ *and* $\sigma > 3/2$*, there exists neighbourhoods* $\mathcal{V}_\sigma$ *and* $\mathcal{V}^\pm$ *of* $(0,0)$ *in* $\mathcal{S}_\sigma$ *such that if* $A = \Psi(U_0, z_0)$ *with* $(U_0, z_0) \in \mathcal{V}_\sigma$*, there exist* $(V_{\pm\infty}; z_{\pm\infty}) \in \mathcal{V}^\pm$ *with* $|V_{\pm\infty} - U_0| \leq C\|z_0\|^2_{H^s_\sigma}$*,* $\|z_{\pm\infty} - z_0\|_{H^s_\sigma} \leq C\|z_0\|^2_{H^s_\sigma}$ *such that for all* $t \in \mathbb{R}$

$$\psi(t) = e^{-\mathrm{i}tE(V_{\pm\infty})} S(V_\pm(t)) + e^{JtE(V_{\pm\infty})} e^{JtH(V_{\pm\infty})} z_{\pm\infty} + \varepsilon_\pm(t)$$

with

$$\begin{aligned}
\left|\dot{V}_\pm(t) + \mathrm{i}\left(E(V_\pm(t)) - E(V_{\pm\infty})\right)\right| &\leq \frac{C}{\langle t\rangle^2}\|z_0\|^2_{H^s_\sigma}, \\
|V_\pm(t) - V_{\pm\infty}| &\leq \frac{C}{\langle t\rangle}\|z_0\|_{H^s_\sigma}, \\
\max\left\{\|\varepsilon_\pm(t)\|_{H^s},\ \|\varepsilon_\pm(t)\|_{H^s_{-\sigma}}, \|\varepsilon_\pm(t)\|_{B^\beta_{\infty,2}}\right\} &\leq \frac{C}{\langle t\rangle^2}\|z_0\|^2_{H^s_\sigma} \\
\text{and } \left\|e^{-JtH(V_{\pm\infty})} e^{J\int_0^t (E(V_\pm(s)) - E(V_{\pm\infty})\, ds} \varepsilon_\pm(t)\right\|_{H^s_{\frac{3}{2}}} &\leq \frac{C}{\langle t\rangle^{\frac{1}{2}}}\|z_0\|^2_{H^s_\sigma}.
\end{aligned}$$

Moreover, the maps $(U_0; z_0) \in \mathcal{V}_\sigma \mapsto (V_{\pm\infty}; z_{\pm\infty}) \in \mathcal{V}^\pm$ *are bijective.*

References

[Bou06a] N. Boussaïd. “Étude de la stabilité des petites solutions stationnaires pour une classe déquations de Dirac non linéaires”. July 2006. URL: http://tel.archives-ouvertes.fr/tel-00108459/PDF/These.pdf.

[Bou06b] N. Boussaïd. " Stable directions for small nonlinear Dirac standing waves " . In: *Comm. Math. Phys.* 268.3 (2006), pp. 757–817. DOI: 10.1007/s00220-006-0112-3. URL: http://hal.archives-ouvertes.fr/hal-00016041/PDF/Article-StabilizationSmallDirac%20SolitonNonResonantCaseFinal.pdf.

[Bou07] N. Boussaïd. *A stability result for small stationary solutions of a class of nonlinear Dirac equations*. 2007. URL: http://basepub.dauphine.fr/xmlui/handle/123456789/6543.

[Bou08] N. Boussaïd. " On the asymptotic stability of small nonlinear Dirac standing waves in a resonant case " . In: *SIAM J. Math. Anal.* 40.4 (2008), pp. 1621–1670. DOI: 10.1137/070684641. URL: http://hal.archives-ouvertes.fr/hal-00116269/PDF/Article-2-StabilizationSmallDir%20acSolitonResonantCaseFinal41.pdf.

[JK79] A. Jensen and T. Kato. " Spectral properties of Schrödinger operators and time-decay of the wave functions ". In: *Duke Math. J.* 46.3 (1979), pp. 583–611.

[KT98] M. Keel and T. Tao. " Endpoint Strichartz estimates ". In: *Amer. J. Math.* 120.5 (1998), pp. 955–980. URL: http://muse.jhu.edu/journals/american_journal_of_mathematics/v120/120.5keel.pdf.

Part III

Results

This part is the content of my work since my PhD thesis.

The order of the chapters is almost chronological in the sense that they are ordered with respect to the age of my first work in the corresponding area. I only swapped the last two chapters. For practical reasons, I've chosen in each chapter to reorder the corresponding works irrespectively of the chronology.

The chapters are presented with the following order in mind:

- From linear to non-linear;
- From time independent to time dependent.

Although the chapters look different, there are common tools and methods. In many respects, the time independent linear theory is present and the properties of the resolvent operator and estimates based on commutator methods are the core of most all these works.

My original field of research is the asymptotic stability of non-linear dispersive equations. The analysis of such problems is at the interface of the spectral theory and non-linear partial differential equations. The idea is to solve some well chosen Cauchy problems in a suitable functional setting. This setting is determined by the spectral and the dispersive properties of an underlying linear problem. I was hence brought up to analyse point spectrum, dispersive properties, non-autonomous Cauchy problems in order to understand the asymptotic stability.

The direct or indirect applicability of the solutions to theses problems to the asymptotic stability problem is a work in progress. The question of spectral and asymptotic stability in non-linear Dirac equations is a promising field with many interesting open problems, see for instance the final report of the focus research group [Bou+12], that we organized in BIRS centre (Banff, Alberta).

References

[Bou+12] N. Boussaïd, A. Comech, S. Gustafson, S. Ibrahim, T. Mizumachi, K. Nakanishi, and A. Stefanov. *Spectral and asymptotic stability of nonlinear Dirac equation.* Tech. rep. 2012. URL: http://www.birs.ca/events/2012/focussed-research-groups/12frg188.

III.4

Spectral pollution

In this section, we present the analysis of [BB10; BBL12; BBBa; BBBb]. The results we have obtained in these works are either properties on the spectral pollution in itself viewed as spectral phenomenon or analysis and implementations of numerical methods that are free from any spectral pollution.

4.1 Introduction

The spectral pollution is a theoretical phenomenon that arises in the numerical computation of self-adjoint operator spectra acting on a separable infinite dimensional Hilbert space $\mathcal{H}$.

Consider λ an isolated eigenvalue of $(A, D(A))$, a self-adjoint operator on $\mathcal{H}$ with domain $\mathrm{D}(A)$, which has an infinite number of spectral values above it and an infinite number of spectral values below, in the sense that $\inf \sigma_{\mathrm{ess}}(A) < \lambda < \sup \sigma_{\mathrm{ess}}(A)$ or, more generally, in the sense that*

$$\operatorname{tr} \mathbb{1}_{(-\infty,\lambda)}(A) = \operatorname{tr} \mathbb{1}_{(\lambda,\infty)}(A) = \infty. \tag{4.1}$$

The numerical estimation of λ constitutes a serious challenge in applied spectral theory. Classical approaches, such as the Galerkin method, suffer from variational collapse under no further restrictions on the approximating space. This often leads to numerical artefacts which do not belong to the spectrum of A, giving rise to what is generically called *spectral pollution*. This can be illustrated by means of the following simple example.

Example 4.1. *Let* $\mathcal{H} = \mathrm{Span}\{e_n^\pm\}_{n\in\mathbb{N}}$ *where* $e_n^\pm$ *is an orthonormal set of vectors in a given scalar product. Let* $\mathcal{L}_n = \mathrm{Span}\{e_1^\pm, \dots, e_{n-1}^\pm, f_n\}$ *where* $f_n = (\cos\theta)e_n^+ + (\sin\theta)e_n^-$ *for* $\theta \in (0, \pi/2)$. *Let*†

$$A = \sum_{n\geq 1} |e_n^+\rangle\langle e_n^+|,$$

that is, A is the orthogonal projector onto $\mathrm{Span}(e_n^+)$ *and* $\sigma(A) = \sigma_{ess}(A) = \{0, 1\}$. *Then* $\sigma(A_n) = \{0, 1, \cos^2\theta\}$ *for all n. Thus imposing $\theta = \frac{\pi}{4}$ will lead to $\frac{1}{2} \in \sigma(A_n)$ for all n while it is not in the spectrum of A.*

Notice that if A has only finitely many eigenvalues with finite multiplicities and is bounded from below, then the characterisation of the discrete spectrum by means of the min-max principle ensures that the Galerkin method is free from any pollution, see Section A.3. So the spectral pollution appears only for operators which are strongly

*For $\mathcal{I} \subset \mathbb{R}$ an interval let $\mathbb{1}_{\mathcal{I}}(A)$ be the spectral projector of A associated to $\mathcal{I}$.

†The bra-ket notation $|f\rangle\langle g|$ denotes the linear operator $\psi \mapsto \langle g, \psi\rangle f$.

indefinite[‡] or in the gap of the essential spectrum. The later should be considered in a generalised sense including $\pm\infty$ whenever there are eigenvalues tending to $\pm\infty$, see condition (4.1).

The spectral pollution phenomenon occurs in different practical contexts such as Sturm-Liouville operators [AGM06; SW95; SW93], perturbations of periodic Schrödinger operators [BL07; Mar10] and systems underlying elliptic partial differential equations [AFW10; BBG98; BBG00]. It is a well-documented difficulty in quantum chemistry and physics, in particular regarding relativistic computations [Kut84; SH84; Gra82; DG81]. It also plays a fundamental role in elasticity and magnetohydrodynamics [KLT04; DS02; Rap+97; Atk+94].

In our analysis of spectral pollution problems, we have adopted two different approaches:

1. analyse and produce numerical methods for strongly indefinite operators (e.g. Dirac, Maxwell) that are free from spectral pollution ;

2. analyse the spectral pollution as a spectral phenomenon in order to understand how it occurs and to localise it.

The first aspect appeared in [BB10] where we considered the second order spectrum for Dirac operators and in [BBBa; BBBb] where we analyse and extend the Lehmann-Maehly-Goerisch and Davies-Plum methods for approximating the spectrum of Maxwell operators in bounded domain. The second aspect was considered in [BBL12] where we obtained a Weyl-type theorem for the spectral pollution.

4.2 A brief chronological description of my work on spectral pollution

From a chronological point of view, the first of my works in these research field was [BB10]. In this analysis, we implemented a certified pollution free method, the quadratic projective method, for Dirac type problems in dimension 3. Unlike the Galerkin method, it is guaranteed to be free from any pollution. Nonetheless the question of the pollution of Galerkin methods with the basis we choose, namely Hermite functions, can be asked and the answer is not trivial. For instance our numerical experiments did not show pollution as long as the basis is balanced with respect to the four components (namely the number of degree of freedom used to approximate each component is the same). The pollution appears when we try to take advantage of the unbalanced character of the eigenvectors (some components are smaller than the others). Although it may seem artificial to unbalance the basis, the problem that we were trying to solve was to improve accuracy given a fixed number of degrees of freedom.

So a natural question arose: does the balanced Hermite basis pollute the spectrum of Dirac type operators ? This lead us to refinements in [BBL12] of the work by Lewin and Séré [LS10]. Indeed with a balanced basis, the analysis in [LS10] ensures that the pollution is absent in the free case. It is then natural to look for conditions that guarantees the stability of pollution by perturbations. The question was solved for operators bounded from below but remains open for the operators which are strongly indefinite. In the case of strongly indefinite operators, we failed to obtain a reasonable “symmetric” mapping theorem, see Theorem 4.9.

We shall also point out that the Galerkin methods do not provide any enclosure for strongly indefinite operators. They are a priori unhierarchical for strongly indefinite

[‡]Strongly indefinite operators are operators unbounded from above and from below.

operators. Indeed the resulting approximations of the eigenvalues are not guaranteed to be upper or lower bounds of the corresponding eigenvalue even if they are free from any pollution. In this respect one can also consider the application of quadratic projective methods to operators which are bounded from below, this has been for instance considered by Boulton and Hobiny [BH13a] (they also considered in [BH13b] application to this context of the method by Zimmermann-Mertins, see Section 4.5). Since a weak formulation of the spectral problem exists for these operators the enclosure obtained by a quadratic projective method has a price which is to double the regularity of the Galerkin basis.

My most recent work on the spectral pollution is an analysis of another method based on finite elements which is free from spectral pollution [BBBa] and its application to the Maxwell operator in a bounded domain [BBBb] in a very low regular setting. The domain even if it is polygonal (2D) or polyhedral (3D) is not necessarily Lipschitz and the permeabilities or permitivities can be rough. The only constraint is that on the solenoidal space the Maxwell operator has compact resolvent. This seems to be true at very high level of generality and is subject to further work with G. Barrenechea and L. Boulton [BBBc]. The numerical method we considered is based on an upper approximation of the spectral distance and its link with a weak spectral formulation introduced by Zimmermann and Mertins [ZM95].

The organization of this section: We start describing, the results on [BBL12] as it contains many interesting statements on the spectral pollution that may be helpful to understand the other analysis.

4.3 Weyl-type results for the non-linear Dirac equation

We present here our analysis [BBL12] of the spectral pollution. These work was lead in the spirit of [LS10] but with a more abstract point view. We studied the stability of the spectral pollution with respect to perturbations in order to locate it and somehow to avoid it.

The ideas was to establish an abstract framework for spectral pollution in the Galerkin method and examine its invariance under relatively compact perturbations. We considered a self-adjoint operator A with domain $\mathrm{D}(A)$ together with $\mathcal{L} = (\mathcal{L}_n)_{n\in\mathbb{N}}$ a sequence of finite dimensional subspaces of $\mathrm{D}(A)$, dense in the graph norm as $n \to \infty$ in the sense of

Definition 4.2 (A-regular Galerkin sequences)**.** *We say that $\mathcal{L} = (\mathcal{L}_n)$, $\mathcal{L}_n \subset \mathrm{D}(A)$, is an* A-regular Galerkin sequence*, or simply an A-regular sequence, if for all $f \in \mathrm{D}(A)$ there exists a sequence of vectors (f_n) with $f_n \in \mathcal{L}_n$ such that $f_n \to f$ in the graph norm of A, that*

$$\|f_n - f\| + \|Af_n - Af\| \to_{n\to\infty} 0.$$

When A is semi-bounded, we also considered a slightly more general framework, which covers important applications such as many of those involving the finite element method. In this framework we will only require that the subspaces $\mathcal{L}_n$ lie in the domain of the quadratic form associated to A and that the sequence $\mathcal{L}$ is dense in the form sense.

Notations : The weak limit is be denoted by $\rightharpoonup$. The ideal of compact operators on $\mathcal{H}$ is be denoted by $\mathcal{K}(\mathcal{H})$.

4.3.1 Limiting spectra

If $\pi_n : \mathcal{H} \longrightarrow \mathcal{L}_n$ is the orthogonal projection in the scalar product of $\mathcal{H}$ onto $\mathcal{L}_n$ then the compression of A to $\mathcal{L}_n$ is $A_n = \pi_n A{\restriction}_{\mathcal{L}_n} : \mathcal{L}_n \longrightarrow \mathcal{L}_n$. We defined $\sigma(A, \mathcal{L})$ as the large n limiting set in Hausdorff distance of the Galerkin method spectra $\sigma(A_n)$ in the sense of the

Definition 4.3 (Limiting spectrum). *The* limiting spectrum of A *relative to* $\mathcal{L}$*,* $\sigma(A, \mathcal{L})$*, is the set of all* $\lambda \in \mathbb{R}$ *for which there exists* $\lambda_k \in \sigma(A_{n_k})$ *such that* $n_k \to \infty$ *and* $\lambda_k \to \lambda$ *as* $k \to \infty$*.*

A real number $\lambda \in \sigma(A, \mathcal{L})$ if and only if there exists a sequence $x_k \in \mathcal{L}_{n_k}$ such that $\|x_k\| = 1$ and $\pi_{n_k}(A - \lambda)\, x_k \to 0$ as $k \to \infty$.

We proved that $\sigma(A) \subset \sigma(A, \mathcal{L})$ and since the equality may fail to occur in this identity, an abstract notion of *limiting spectral pollution set* can be formulated naturally as,

$$\sigma_{\mathrm{poll}}(A, \mathcal{L}) = \sigma(A, \mathcal{L}) \setminus \sigma(A).$$

We realised that points in the limiting spectral pollution set can be characterised in a similar fashion as points in the essential spectrum. Therefore a question arose:

> What are the conditions on a perturbation B that ensure $\sigma_{\mathrm{poll}}(A, \mathcal{L}) = \sigma_{\mathrm{poll}}(B, \mathcal{L})$?

Our analysis relied on the characterisation of $\sigma(A, \mathcal{L})$ in terms of special Weyl-type sequences ($\mathcal{L}$-Weyl sequences) and its structural properties. Let us recall the

Definition 4.4 (Limiting essential spectrum). *We denote by* $\sigma_{\mathrm{ess}}(A, \mathcal{L})$ *the set of all* $\lambda \in \sigma(A, \mathcal{L})$ *for which there exists an* $\mathcal{L}$*-Weyl sequence* (x_k) *that is a sequence* $x_k \in \mathcal{L}_{n_k}$ *such that* $\|x_k\| = 1$ *and* $\pi_{n_k}(A - \lambda)\, x_k \to 0$ *as* $k \to \infty$*. such that* $x_k \rightharpoonup 0$.

Thus we could consider a decomposition of $\sigma(A, \mathcal{L})$ as the disjoint union of a *limiting essential spectrum* associated with $\mathcal{L}$, $\sigma_{\mathrm{ess}}(A, \mathcal{L})$, and its *limiting discrete spectrum* counterpart, $\sigma_{\mathrm{disc}}(A, \mathcal{L})$. We showed that the former contains both the true essential spectrum $\sigma_{\mathrm{ess}}(A)$ and $\sigma_{\mathrm{poll}}(A, \mathcal{L})$. Actually we proved that the limiting spectra enjoy the following properties:

(i) the limiting spectrum $\sigma(A, \mathcal{L})$ and the limiting essential spectrum $\sigma_{\mathrm{ess}}(A, \mathcal{L})$ are closed subsets of $\mathbb{R}$;

(ii) moreover $\sigma_{\mathrm{ess}}(A) \subset \sigma_{\mathrm{ess}}(A, \mathcal{L})$ and $\sigma_{\mathrm{disc}}(A, \mathcal{L}) \subset \sigma_{\mathrm{disc}}(A)$.

Hence if $\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(A, \mathcal{L})$ then automatically $\sigma_{\mathrm{disc}}(A) = \sigma_{\mathrm{disc}}(A, \mathcal{L})$ and $\sigma(A) = \sigma(A, \mathcal{L})$.

4.3.2 Stability properties of the limiting essential spectrum

In this part, we only consider semi-bounded operators. We explain in Section 4.3.3 this limitation.

The condition we found to ensure the stability of the spectral pollution

$$\sigma_{\mathrm{ess}}(B, \mathcal{L}) = \sigma_{\mathrm{ess}}(A, \mathcal{L}).$$

on the perturbed operator B with respect to A sums up in

Theorem 4.5 (Weyl-type stability theorem for the limiting spectra)**.** *Let A and B be two self-adjoint operators which are bounded below. Assume that for some $a < \inf\{\sigma(A), \sigma(B)\}$,*

$$\mathrm{D}((B-a)^{1/2}) = \mathrm{D}((A-a)^{1/2}) \tag{4.2}$$

and

$$(A-a)^{1/2}((B-a)^{-1/2} - (A-a)^{-1/2}) \in \mathcal{K}(\mathcal{H}).$$

Then

$$\sigma_{\mathrm{ess}}(A, \mathcal{L}) = \sigma_{\mathrm{ess}}(B, \mathcal{L})$$

for all sequences $\mathcal{L} = (\mathcal{L}_n)$ which are simultaneously $(A-a)^{1/2}$-regular and $(B-a)^{1/2}$-regular.

Hence an approximating sequence $\mathcal{L}$ will not asymptotically pollute for A in a given interval if and only if it does not pollute for B in the same interval. This generalises [LS10, Corollary 2.5].

In order to obtain a more practical statement we provided the

Corollary 4.6. *Let A and B be two bounded-below self-adjoint operators such that (4.2) holds true for some $a < \inf\{\sigma(A), \sigma(B)\}$. Assume that $C := B - A$ is a densely defined symmetric operator such that*

$$C \in \mathcal{B}(\mathrm{D}((B-a)^{\beta}), \mathcal{H})$$

and

$$(A-a)^{-\alpha} C (B-a)^{-\beta} \in \mathcal{K}(\mathcal{H}) \tag{4.3}$$

for some $0 \le \alpha, \beta < 1$ with $\alpha + \beta < 1$. Then

$$\sigma_{\mathrm{ess}}(A, \mathcal{L}) = \sigma_{\mathrm{ess}}(B, \mathcal{L})$$

for all sequences $\mathcal{L} = (\mathcal{L}_n)$ which are simultaneously $(A-a)^{1/2}$-regular and $(B-a)^{1/2}$-regular.

Remark 4.7. *Let A be a given bounded-below self-adjoint operator and assume that A has a gap (a, b) in its essential spectrum in the following precise sense,*

$$\sigma_{\mathrm{ess}}(A) \cap (a, b) = \varnothing, \qquad \mathrm{tr}\left(\mathbb{1}_{(-\infty,a)}(A)\right) = \mathrm{tr}\left(\mathbb{1}_{(b,\infty)}(A)\right) = +\infty.$$

Let $\Pi := \mathbb{1}_{(c,\infty)}(A)$ where $a < c < b$. Results shown in [LS10] ensure that, when the Galerkin spaces $\mathcal{L}_n$ are compatible with the decomposition $\mathcal{H} = \Pi\mathcal{H} \oplus (1-\Pi)\mathcal{H}$ (i.e. when Π and π_n commute for all n), there is no pollution in the gap: $\sigma_{\mathrm{ess}}(A, \mathcal{L}) \cap (a, b) = \varnothing$. According to [LS10, Corollary 2.5], when

$$(B-a)^{-1} C (A-a)^{-1/2} \in \mathcal{K}(\mathcal{H}), \tag{4.4}$$

then $\sigma_{\mathrm{ess}}(B, \mathcal{L}) \cap (a, b) = \varnothing$ as well.

In this respect, Theorem 4.5 can be seen as a generalisation of these results. Although condition (4.3) is stronger than (4.4), the statement guarantees that the whole *polluted spectrum will not move irrespectively of the $(A-a)^{1/2}$-regular Galerkin family $\mathcal{L}$ and not only for those satisfying $[\Pi, \pi_n] = 0$ for all n.* □

Example 4.8 (Periodic Schrödinger operators)**.** *Let $A = -\Delta + V_{\rm per}$ where $V_{\rm per}$ is a periodic potential with respect to some fixed lattice $\mathcal{R} \subset \mathbb{R}^d$ (for instance $\mathcal{R} = \mathbb{Z}^3$). Let $C = W(x)$ be a perturbation. Assume that*

$$V_{\rm per} \in L^p_{\rm loc}(\mathbb{R}^d) \quad \textit{where} \quad \begin{cases} p = 2 & \textit{if } d \leq 3 \\ p > 2 & \textit{if } d = 4 \\ p = d/2 & \textit{if } d \geq 5 \end{cases}$$

and that

$$W \in L^q(\mathbb{R}^d) \cap L^p_{\rm loc}(\mathbb{R}^d) + L^\infty_\epsilon(\mathbb{R}^d)$$

for $\max(d/2, 1) < q < \infty$*. Then (4.3) holds true for suitable α, β and a, and therefore*

$$\sigma_{\rm ess}\left(-\Delta + V_{\rm per} + W, \mathcal{L}\right) = \sigma_{\rm ess}\left(-\Delta + V_{\rm per}, \mathcal{L}\right) \tag{4.5}$$

for all A-regular Galerkin sequence $\mathcal{L}$. See [LS10, Section 2.3.1].

A Galerkin sequence $\mathcal{L}$ which does not lead to any pollution in a given gap, can be found by localised Wannier functions, [LS10; CDL08]. In practice, these functions can only be calculated numerically, so it is natural to ask what would be the polluted spectrum when they are known only approximately. According to (4.5), the polluted spectrum will not increase in size more than that of the unperturbed operator $-\Delta + V_{\rm per}$. □

4.3.3 Mapping of the limiting spectra

Our approach consisted in adapting to the context of limiting spectra, several classical results for the spectrum and essential spectrum. This lead to many unexpected difficulties which were illustrated on a variety of simple examples in [BBL12].

In particular, we established a limiting spectra version of the spectral mapping theorem allowing to replace the unbounded operator A by its (bounded) resolvent $(A - a)^{-1}$.

Theorem 4.9 (Mapping of the limiting spectra)**.** *Let A be semi-bounded from below and let $a < \inf \sigma(A)$. Assume that $\mathcal{L}$ is an $(A - a)^{1/2}$-regular Galerkin sequence. Then*

$$\lambda \in \sigma(A, \mathcal{L}) \quad \Longleftrightarrow \quad (\lambda - a)^{-1} \in \sigma\left((A - a)^{-1}, \mathcal{G}\right)$$

and

$$\lambda \in \sigma_{\rm ess}(A, \mathcal{L}) \quad \Longleftrightarrow \quad (\lambda - a)^{-1} \in \sigma_{\rm ess}\left((A - a)^{-1}, \mathcal{G}\right)$$

where $\mathcal{G} = \left((A - a)^{1/2}\mathcal{L}_n\right)_{n\in\mathbb{N}}$.

Remark 4.10. *Recall that a self-adjoint operator A is unbounded ($\mathrm{D}(A) \subsetneq \mathcal{H}$) if and only if $0 \in \sigma((A - a)^{-1})$ for one (hence for all) $a \notin \sigma(A)$. As it turns out, A is unbounded if and only if $0 \in \sigma_{\rm ess}((A - a)^{-1}, \mathcal{G})$ for one (and hence all) $a < \min \sigma(A)$ and $(A - a)^{1/2}$-regular sequence $\mathcal{L}$. Formally in Theorem 4.9 this corresponds to the case $+\infty \in \sigma(A)$ and $(+\infty - a)^{-1} = 0$.* □

When A is not semi-bounded but its essential spectrum has a gap containing a number a, we could as well consider sequences $(\mathcal{L}_n)$ which are only $|A - a|^{1/2}$-regular. We have chosen to avoid mentioning quadratic forms for operators which are not semi-bounded, because in practical applications (such as those involving the Dirac operator) the domain of $|A - a|^{1/2}$ does not necessarily coincide with the natural domain upon which the quadratic form is defined.

Another apparent reason for why A is required to be semi-bounded, is in order to be able to use a square root $(A - a)^{1/2}$ in the definition of $\mathcal{G}$. But there is a more fundamental reason. When a is in a gap of the essential spectrum, it would be natural to expect an extension of the above result by considering, for example, $\mathcal{G} = \big(|A-a|^{1/2}\mathcal{L}_n\big)_{n\in\mathbb{N}}$. We provided the following simple example showing that this extension is not possible in general.

Example 4.11 (Impossibility of extending Theorem 4.9 for A strongly indefinite)**.** *Let $\mathcal{H} = \mathrm{Span}\{e_n^\pm\}_{n\in\mathbb{N}}$ where $e_n^\pm$ is an orthonormal set of vectors in a given scalar product. Define $\mathcal{L}_n = \mathrm{Span}\{e_1^\pm, \dots, e_{n-1}^\pm, \cos(\theta_n)\, e_n^+ + \sin(\theta_n)\, e_n^-\}$ with $\theta_n := \pi/4 - \lambda/(2n)$ for a fixed $\lambda \in (0,1)$. Let*

$$A = \sum n|e_n^+\rangle\langle e_n^+| - \sum n|e_n^-\rangle\langle e_n^-|.$$

Then $\sigma(A) = \{\pm n : n \in \mathbb{N}\} = \sigma_{\mathrm{disc}}(A)$. On the other hand

$$\sigma(A,\mathcal{L}) = \sigma(A)\cup\{\lambda\}, \qquad \sigma_{\mathrm{ess}}(A,\mathcal{L}) = \{\lambda\} \quad \textit{and} \quad \sigma_{\mathrm{disc}}(A,\mathcal{L}) = \sigma(A).$$

Now

$$A^{-1} = \sum n^{-1}|e_n^+\rangle\langle e_n^+| - n^{-1}|e_n^-\rangle\langle e_n^-|$$

and $\mathcal{G} = \sqrt{|A|}\mathcal{L} = \mathcal{L}$. Since A^{-1} is compact we have

$$\sigma(A^{-1},\mathcal{G}) = \sigma(A^{-1}) \quad \textit{and} \quad \sigma_{\mathrm{ess}}(A^{-1},\mathcal{G}) = \sigma_{\mathrm{ess}}(A^{-1}) = \{0\}.$$

Thus $\lambda \in \sigma_{\mathrm{ess}}(A,\mathcal{L})$ whereas $1/\lambda \notin \sigma(A^{-1},\mathcal{G})$. □

We also provided a counter-example when a is chosen in the the convex hull of the spectrum.

4.4 The quadratic projection method for the Dirac operator

We now present the analysis [BB10] of our implementation of the quadratic projective method to the case of the Dirac operator.

As already mentioned in the previous section, the Galerkin methods may lead to a variational collapse when A is strongly indefinite. In the case where the operator is semi-bounded these methods relies on the min-max principle, see Section A.3, which shows that they are hierarchical. This principle also reveals a drawback of these methods. Any eigenvalue in a gap of the essential spectrum cannot be attained as the methods stops at the lowest (or highest) threshold of the essential spectrum.

A simple idea can change the situation, if λ is an eigenvalue of A then $|\lambda-\mu|$ is an eigenvalue of $|A-\mu|$. So that a Galerkin method will give access to the eigenvalues in a vicinity of μ. The story is not that simple as the "oscillations" of the eigenvectors will deteriorate the situation compared to the original case but the main issue is the absolute value. To get ride of this difficulty then one can try to consider the square as $(\lambda-\mu)^2$ is an eigenvalue of $(A-\mu)^2$.

For semi-bounded operators there is a weak formulation for the associated eigenvalue problem. Therefore the idea we just mention doubles the cost of the method. For a strongly indefinite operator, this does not change much. This was one of the justification for the analysis we present here.

4.4.1 The second order spectrum

The second order spectrum is the core notion of the quadratic projection method, it was introduced by Davies in [Dav98, Section 9]. The aim of the quadratic projection method is to compute the *second order spectrum of A relative to $\mathcal{L}$*, some finite dimensional space.

Let $\mathcal{L} \subset \mathrm{D}(A)$ be a fixed subspace of finite dimension:

$$\mathcal{L} = \mathrm{Span}\{b_1, \dots, b_n\}$$

where the vectors b_j are linearly independent, define

$$\begin{aligned} K := (\langle Ab_j, Ab_k \rangle)_{j,k=1}^n, \qquad L := (\langle Ab_j, b_k \rangle)_{j,k=1}^n \\ \text{and} \qquad B := (\langle b_j, b_k \rangle)_{j,k=1}^n. \end{aligned} \tag{4.6}$$

and for $z \in \mathbb{C}$, let

$$Q(z) := Bz^2 - 2zL + K \in \mathbb{C}^{n \times n}.$$

The *second order spectrum of A relative to $\mathcal{L}$* is defined by

$$\sigma_2(A, \mathcal{L}) := \sigma(Q) = \{\lambda \in \mathbb{C} \,:\, Q(\lambda)\underline{v} = 0, \text{ some } 0 \neq \underline{v} \in \mathbb{C}^n\}.$$

Since B is a non-singular matrix, $\sigma_2(A, \mathcal{L})$ consists of at most $2n$ points. These points do not lie on the real line, except if $\mathcal{L}$ contains eigenvectors of A. However, since $Q(z)^* = Q(\overline{z})$,

$$\overline{\sigma_2(A, \mathcal{L})} = \sigma_2(A, \mathcal{L}).$$

4.4.2 The quadratic projective method

The quadratic projective method aims at approximating the discrete spectrum of A using the second order spectrum, this was for instance discussed in [LS04], [Bou07], [BL07] and the references therein. The connection between $\sigma(A)$ and $\sigma_2(A, \mathcal{L})$ is the content of

Theorem 4.12. *[BB10, Theorem 1] Let $\mathcal{L} \subset \mathrm{D}(A)$ be finite-dimensional. If $\lambda \in \sigma_2(A, \mathcal{L})$, then*

$$[\Re(\lambda) - |\Im(\lambda)|, \Re(\lambda) + |\Im(\lambda)|] \cap \sigma(A) \neq \varnothing. \tag{4.7}$$

Moreover, suppose that E is an isolated eigenvalue of A with associated eigenspace $\mathcal{E} \subset \mathrm{D}(A)$. Let

$$d_E := \mathrm{dist}(E, \sigma A \setminus \{E\}) = \min\{|E - x| \,:\, x \in \sigma(A),\, x \neq E\}.$$

If

$$[\Re(\lambda) - |\Im(\lambda)|, \Re(\lambda) + |\Im(\lambda)|] \cap \sigma(A) = \{E\}$$

and $Q(\lambda)\underline{v} = 0$ for $0 \neq \underline{v} \in \mathbb{C}^n$, then the corresponding $v \in \mathcal{L}$ satisfies

$$\frac{\|v - \Pi_{\mathcal{E}} v\|}{\|v\|} \leq \frac{\sqrt{2}|\Im\lambda|}{d_E}. \tag{4.8}$$

There is no concern with the position of E relative to the essential spectrum, or any semi-definitness condition imposed on A. The procedure is always free from spectral pollution.

Out of this theorem, we produced, in [BB10], the following procedure for estimating $\sigma(A)$ from the points in $\sigma_2(A, \mathcal{L})$

Procedure 4.4.1. *Quadratic projection method*

- *Choose a suitable* $\mathcal{L} \subset \mathrm{D}(A)$ *;*
- *Find* $Q(z)$ *(compute* $\sigma_2(A, \mathcal{L})$*) ;*
- *The* $\lambda \in \sigma_2(A, \mathcal{L})$ *which are close to* $\mathbb{R}$ *will necessarily be close to* $\sigma(A)$*, if* λ *is close enough to an isolated eigenvalue* E *of* A*, then*

$$|\Re\lambda - E| \leq |\Im\lambda| \tag{4.9}$$

and an associated vector $0 \neq v \in \mathcal{L}$ *(such that* $Q(\lambda)\underline{v} = 0$*) approaches the eigenspace associated to this eigenvalue with an error also determined by* $|\Im(\lambda)|$*.*

The convergence of the method will be ensured if we consider an A^2-regular Galerkin sequence of subspaces $\mathcal{L}_n$, see Definition 4.2, as stated in

Theorem 4.13. *[Bou07, Theorem 2.1] see [BB10, Theorem 2] Let* λ *be an isolated eigenvalue of finite multiplicity of* A *with associated eigenspace denoted by* $\mathcal{E}$*. Suppose that* $\mathcal{L}_n \subset \mathrm{D}(A^2)$ *is a sequence of subspaces such that*

$$\|A^p(u - \Pi_n u)\| \leq \delta(n)\|u\| \qquad \forall u \in \mathcal{E},\ p = 0, 1, 2,$$

where $\delta(n) \to 0$ *as* $n \to \infty$ *is independent of* u *and* p*. Then there exists* $b > 0$ *and* $\lambda_n \in \sigma_2(A, \mathcal{L}_n)$*, such that*

$$|\lambda_n - \lambda| < b\delta(n)^{1/2}. \tag{4.10}$$

Hence if $\mathcal{L}_n$ is an A^2-regular Galerkin sequence then one can find points of $\sigma_2(A, \mathcal{L})$ near the real axis. This guarantees the existence of a sequence $\lambda_n \in \sigma_2(A, \mathcal{L}_n)$ accumulating at points of the *discrete* spectrum of A.

4.4.3 Application to the radial Dirac operator

The main purpose of our analysis was to obtain an efficient pollution free method for a class of Dirac operator. We restricted our analysis to the spherically symmetric case and took advantage of the radial reduction. So, instead of the Dirac operator, we considered the operator H_κ, see (2.5). The radial reduction being all of the same type for any dimension another advantage was that the method applies to any dimension but 1. The latter can be included.

Once the method properties were established, the analysis was reduced to a proper choice of some H_κ^2-regular Galerkin sequence.

We considered $\mathcal{M}_N \subset L^2(0, \infty)$ a nested family of finite-dimensional subspaces such that $\mathcal{M}_N \subset \mathcal{M}_{N+1}$,

$$\overline{\bigcup_{N \geq 1} \mathcal{M}_N} = L^2(0, \infty)$$

and $\mathcal{L}_{NM} := \mathcal{M}_N \oplus \mathcal{M}_M \subset \mathrm{D}(H_\kappa)$. Then $\mathcal{L}_{NM} \subset \mathrm{D}(H_\kappa)$ were chosen as the one generated by odd Hermite functions:

$$\Phi_k(r) := c_{2k+1}^{-1} h_{2k+1}(r) e^{-\frac{r^2}{2}}, \qquad r \geq 0, \qquad k \geq 0,$$

where $h_n(r)$ are the Hermite polynomials and $c_n = \sqrt{2^{n-1} n! \sqrt{\pi}}$ are normalisation constants. More precisely

$$\mathcal{L} \equiv \mathcal{L}_{NM} := \mathrm{Span}\left\{ \begin{pmatrix} \Phi_1(r) \\ 0 \end{pmatrix}, \ldots, \begin{pmatrix} \Phi_N(r) \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \Phi_1(r) \end{pmatrix}, \ldots, \begin{pmatrix} 0 \\ \Phi_M(r) \end{pmatrix} \right\}. \tag{4.11}$$

We considerer balanced ($N = M$) and unbalanced ($N \neq M$) number of basis elements in the first and second component.

The odd-order Hermite functions are the normalised wave functions of a harmonic oscillator,

$$-\Phi_k''(r) + r^2\Phi_k(r) = (4k+3)\Phi_k(r),$$

subject to Dirichlet boundary condition at the origin. They form an orthonormal basis of $L^2(0,\infty)$ and so $B = I$ in (4.6). The entries of the other matrices K and L in (4.6) can also be found explicitly from known properties of the Hermite polynomials, see [BB10, Table 1 & 2].

As the Hermite polynomials are eigenvectors of the Harmonic oscillator, we introduced

$$A = \begin{pmatrix} \tilde{A} & 0 \\ 0 & \tilde{A} \end{pmatrix}$$

where $\tilde{A} = -\partial_r^2 + r^2$ acting on $L^2(0,\infty)$, subject to Dirichlet boundary conditions at the origin.

If $\phi_{\text{sc,el,am}} \in C^\infty(0,\infty)$ are such that $r \mapsto r^\alpha \phi_{\text{sc,el,am}}(r)$ are locally bounded for some $\alpha \in (0,1)$. Then we verified that we have an H^2_κ-regular Galerkin sequence. Hence for any isolated eigenvalue E of H_κ with finite multiplicity and associated eigenspace $\mathcal{E}$, there exist $b_{\text{u}}, b_{\text{l}} > 0$ independent of N or M, and a sequence $\lambda_{NM} \in \sigma_2(H_\kappa, \mathcal{L}_{NM})$, such that

$$|\lambda_{NM} - E| < b_{\text{u}} N^{-\frac{q_{\text{l}}-1}{2}} + b_{\text{l}} M^{-\frac{q_{\text{l}}-1}{2}} \qquad \text{and } \|(I - \Pi_{\mathcal{E}})v_{NM}\| < b_{\text{u}} N^{-\frac{q_{\text{u}}-1}{2}} + b_{\text{l}} M^{-\frac{q_{\text{l}}-1}{2}}$$

for $1 < q_{\text{u}} = q_{\text{l}} < 5/4$ and v_{NM} an eigenvector of $Q(\lambda_{NM})$.

4.4.4 Upper/lower spinor component balance and approximation of eigenvalues

We have implemented different numerical experiments that were added to the collection [Bet+13]. We refer to our published analysis [BB10] for a complete description. Let us just mention the outcome of the experiments with unbalanced basis. The previous paragraph may suggest that an optimal rate of approximation might be achieved by choosing an equal number of upper/lower spinor components in (4.11). Contrary to this presumption, and depending on the potential V, the numerical evidence we obtained showed that the residual on the right side of (4.9) can in some cases decrease significantly by suitably choosing $N \neq M$.

In Figure 4.1, we have performed the following experiment. Fix the number of degrees of freedom, $\dim(\mathcal{L}_{MN}) = 200$. Then for $N = 10:5:190$ and $M = 200 - N$, use the quadratic method as well as the Galerkin method to approximate eigenvalues of H_κ in the spectral gap $(-1,1)$.

We firstly considered $\phi_{\text{sc}} = \phi_{\text{am}} = 0$ and $\phi_{\text{el}}(r) = -1/(2r)$. The Galerkin method might or might not produce spurious eigenvalues. The quadratic method will always provide two-sided non-polluted bounds for the true eigenvalues with a residual, obtained from (4.7), which might change with N. See also figures 4.3 and 4.4 (left). The Galerkin method appeared to pollute heavily near the upper end of the gap for $N > M$. Moreover, for the ground state, the minimal $|\Im(\lambda)|$ is not achieved at $N = 100$ which corresponds to $N = M$, but rather at some $N > 100$. Remarkably, the residual are reduced significantly (up to 66% for the true residual) when $M(N)/N \approx 1/5$.

We performed the analogous experiment for the inverse harmonic potential $\phi_{\text{el}}(r) = \gamma/(1+r^2)$, the conclusion were also rather surprising. See Figure 4.2. The Galerkin method

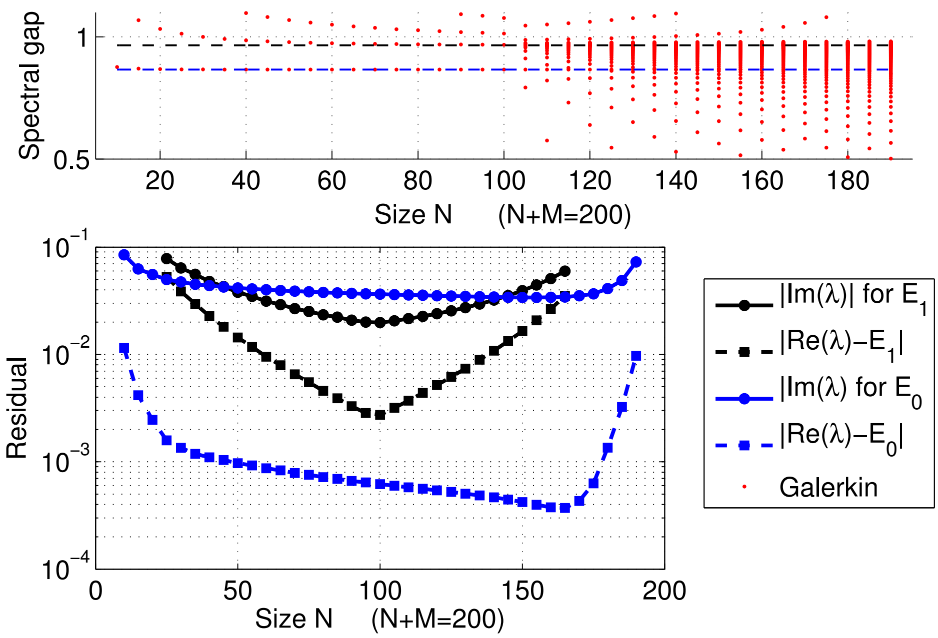

Figure 4.1: Here E_0 and E_1 are eigenvalues of H_{-1} for $\phi_{\rm el}(r) = -\frac{1}{2r}$. The top graph shows the eigenvalues of L in (4.6) (that is the Galerkin approximation) for $G = H_{-1}$ and $(M, N) = (N, 200 - N)$ so that $\dim(\mathcal{L}_{NM}) = 200$. The bottom graph depicts the residuals $|\Im(\lambda)|$ and $|\Re(\lambda) - E_j|$. For E_0, the minimum of the residual curve corresponding to $|\Im(\lambda)|$ is achieved when $N \approx 155$ and it is roughly 7% smaller than when $N = 100$. For the same eigenvalue, the residual curve corresponding to $|\Re(\lambda) - E_0|$ achieves its minimum when $N = 165$ and it is roughly 66% smaller than when $N = 100$.

appeared to pollute heavily near the upper end of the gap for $N > M$. However, now the approximation is improved by over 16% for E_0 and over 18% for E_1, if $M(N)/N \approx 3$.

The above phenomena is related to the fact that the constants $b_{\rm u}$ and $b_{\rm l}$ in the previous paragraph do not need to be close to each other. It can be explained by considering the relation between the components of the exact eigenvectors, we refer to [BB10, Section 4.4].

N	a	b
$n/8$	-0.6736	1.6766
$n/4$	-0.5426	0.6555
$3n/8$	-0.4385	0.3530
$n/2$	-0.3963	0.2703
$5n/8$	-0.5064	0.4478
$3n/4$	-0.6903	1.1115
$7n/8$	-0.9609	5.4520

N	a	b
$n/8$	-1.3241	8.8276
$n/4$	-0.9135	1.1303
$3n/8$	-0.7990	0.7223
$n/2$	-0.7979	0.8155
$5n/8$	-0.8125	1.0825
$3n/4$	-0.8163	1.5171
$7n/8$	-0.8004	2.4558

Table 4.1: In this table we fit by least squares the data of Figure 4.4 and find a and b such that $|\lambda_n - E_0| \leq |\Im(\lambda_n)| \sim bn^a$ for $n = N + M$.

4.4.5 A comment on the Galerkin method in the balanced case

Strong numerical evidence suggests that (for any of the potentials considered above) no spurious eigenvalue is produced by the Galerkin method when $N = M$. It may be surprising to consider a more complicated procedures, such as the quadratic projection

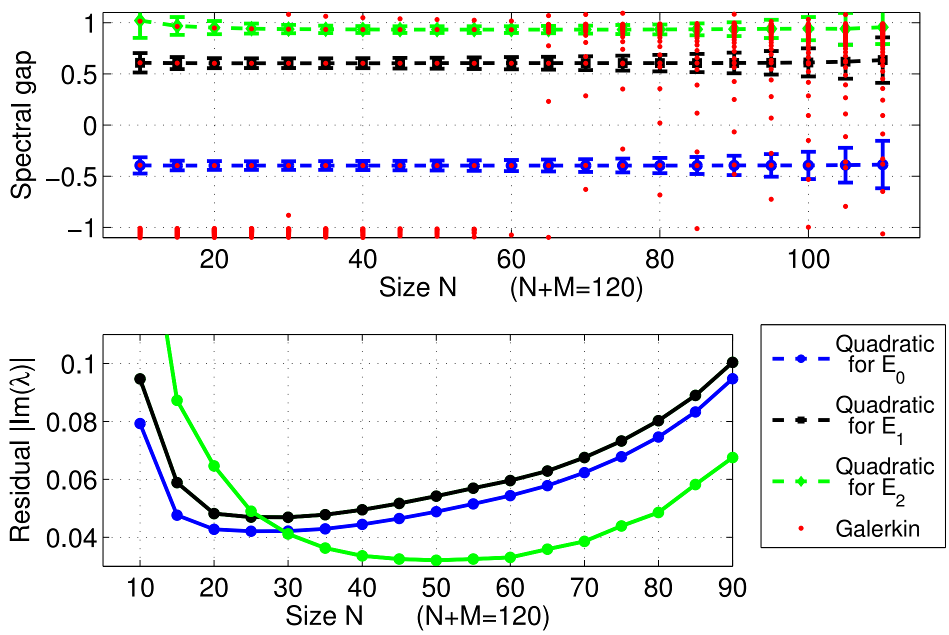

Figure 4.2: Here E_0, E_1 and E_2, are the first three eigenvalues of H_{-1} for $\phi_{\rm el}(r) = -4/(1+r^2)$. The top graph shows approximation of $E_0 \approx -0.3955$, $E_1 \approx 0.6049$ and $E_2 \approx 0.9328$, for $(M,N) = (N, 120-N)$ so that $\dim(\mathcal{L}_{NM}) = 120$. The curves correspond to $\Re(\lambda_n)$ for $\lambda = \lambda_n$ in (4.8) and (4.10). The vertical bars measure $|\Im(\lambda_n)|$. The image is superimposed with the eigenvalues of L in (4.6) for $G = H_{-1}$, that is the Galerkin approximation. The bottom graph depicts the residuals $|\Im(\lambda_n)|$.

method, to avoid inexistent spectral pollution. But, on the one hand, the quadratic projective method is robust: as a priori it is quite unclear whether the Galerkin method pollutes for a given basis or not. On the other hand, as the experiments of this section suggest, some times forcing pollution into a model might improve convergence properties.

Nonetheless, understanding whether or not the Galerkin method for a balanced basis pollutes is a difficult problem which lead to the analysis [BBL12]. But the problem is still open.

4.5 Pollution-free methods for the Maxwell operator

We present here two analysis [BBBa; BBBb] on which we improved and implemented another pollution free method originated from Lehmann-Maehly-Goerisch method [GA86; Wei74], later extended by Zimmermann and Mertins [ZM95] and then developed by Davies and Plum [DP04].

The approach of Zimmermann and Mertins is based on an extension of the Lehmann-Maehly-Goerisch method [GA86; Wei74] and it has proved to be highly successful in concrete numerical implementations: computation of bounds for eigenvalues of the radially reduced magnetohydrodynamics operator [ZM95; BS12], complementary eigenvalue bounds for the Helmholtz equation [BM01] and calculation of sloshing frequencies in the left definite case [Beh09].

Our analysis was initiated with the results presented in [DP04, Section 6] where it is shown that their techniques based on a notion of approximated spectral distance is equivalent to the one initiated by Zimmermann and Mertins.

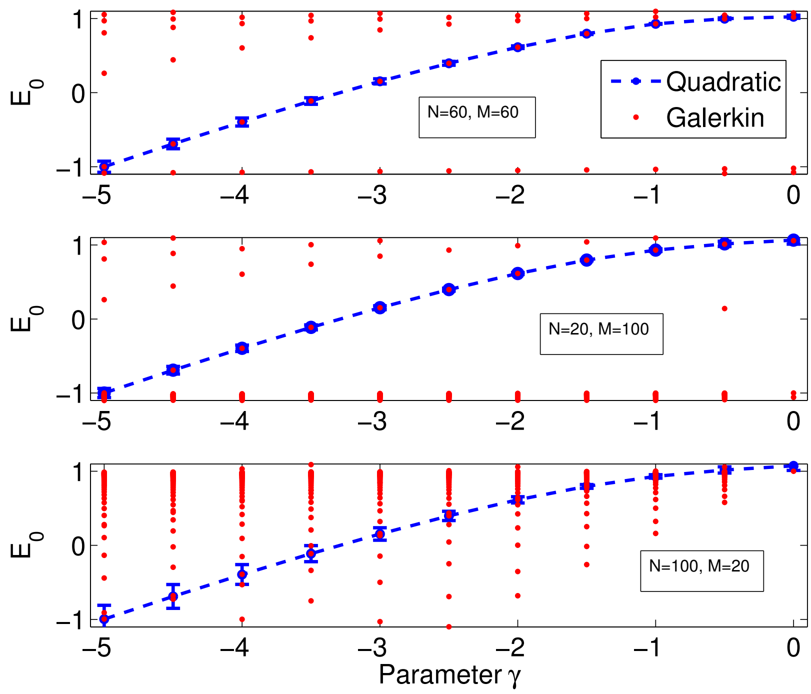

Figure 4.3: The graph captures the evolution of E_0 as it crosses the spectral gap of H_{-1} where $\phi_{\rm el}(r) = \gamma/(1+r^2)$ for $\gamma = -5 : .5 : 0$. We consider three choices of pairs (N, M) such that $\dim(\mathcal{L}_{NM}) = 120$. The curve corresponds to $\Re(\lambda_n)$ for $\lambda = \lambda_n$ in (4.8) and (4.10). The vertical bars on the curve measure $|\Im(\lambda_n)|$. We superimpose the image with the eigenvalues of L in (4.6) for $G = H_{-1}$, that is the Galerkin approximation.

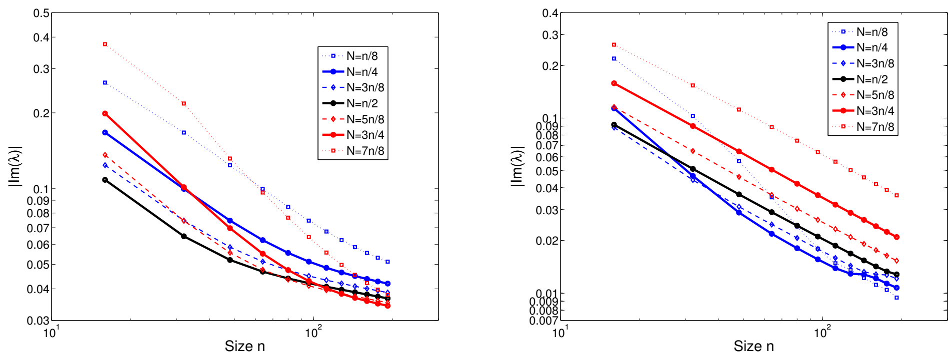

Figure 4.4: Log-log plots of $|\Im(\lambda)|$ for $\Re(\lambda)$ close to an eigenvalue, E_0, for different choices of pairs (N, M) as $n = N + M$ increases. Left: $\kappa = -1$, $\phi_{\rm el}(r) = -\frac{1}{2r}$ and $E_0 \approx 0.86602$. Right: $\kappa = -1$, $\phi_{\rm el}(r) = -\frac{2}{1+r^2}$ and $E_0 \approx 0.61399$. See Table 4.1.

We determined in a more precise manner the nature of this equivalence and examine their convergence properties.

We extended various canonical results from [DP04]. Notably, we included multiplicity counting and a description of how eigenfunctions are approximated. We also addressed the questions of convergence and upper bounds for residuals in both methods.

Notations : For J a Borel subset of $\mathbb{R}$, the spectral projector associated to A is denoted by $\mathbb{1}_J(A)$ and $\mathcal{E}_J(A) = \oplus_{\lambda \in J} \operatorname{Ker}(A-\lambda)$[§].

4.5.1 Approximated local counting functions

In order to explain how we included the multiplicities in the original method by [DP04] we explain how we generalised the approximated distance.

First for $t \in \mathbb{R}$, $q_t : \mathrm{D}(A) \times \mathrm{D}(A) \longrightarrow \mathbb{C}$ is the closed bilinear form

$$q_t(u,w) = \langle (A-t)u, (A-t)w \rangle \qquad \forall u, w \in \mathrm{D}(A).$$

We defined the following t-dependant semi-norm, which is a norm if t is not an eigenvalue,

$$|u|_t = q_t(u,u)^{1/2} = \|(A-t)u\|.$$

By virtue of the min-max principle, Section A.3, q_t characterises the spectrum which lies near the origin of the positive operator $(A-t)^2$. This is reminiscent of the quadratic projective method, from previous section. But this gives also rise to a notion of local counting function at t for the spectrum of A as follows. If

$$\mathfrak{d}_j(t) = \inf_{\substack{\dim V = j \\ V \subset \mathrm{D}(A)}} \sup_{u \in V} \frac{|u|_t}{\|u\|}$$

then $0 \le \mathfrak{d}_j(t) \le \mathfrak{d}_k(t)$ for $j < k$.

Now notice that $\mathfrak{d}_1(t)$ is in fact the Hausdorff distance from t to $\sigma(A)$,

$$\mathfrak{d}_1(t) = \min\{\lambda \in \sigma(A) : |\lambda - t|\} = \inf_{u \in \mathrm{D}(A)} \frac{|u|_t}{\|u\|}$$

and similarly $\mathfrak{d}_j(t)$ are the distances from t to the j-th nearest point in $\sigma(A)$ counting multiplicity in a generalised sense. That is, stopping when the essential spectrum is reached.

Consequently it is possible to extract certified information about $\sigma(A)$ in the vicinity of t from the action of A onto finite-dimensional trial subspaces $\mathcal{L} \subset \mathrm{D}(A)$, see [Dav98, Section 3], as follows. For $j \le n = \dim \mathcal{L}$, with

$$F^j_{\mathcal{L}}(t) = \min_{\substack{\dim V = j \\ V \subset \mathcal{L}}} \max_{u \in V} \frac{|u|_t}{\|u\|}.$$

we have $0 \le F^1_{\mathcal{L}}(t) \le \ldots \le F^n_{\mathcal{L}}(t)$ and $F^j_{\mathcal{L}}(t) \ge \mathfrak{d}_j(t)$ for all $j = 1, 2, \ldots, n$. Since $[t - \mathfrak{d}_j(t), t + \mathfrak{d}_j(t)] \subseteq [t - F^j_{\mathcal{L}}(t), t + F^j_{\mathcal{L}}(t)]$, there are at least j spectral points of A in the segment $\left[t - F^j_{\mathcal{L}}(t), t + F^j_{\mathcal{L}}(t)\right]$ including, possibly, the essential spectrum. That is

$$\operatorname{tr} \mathbb{1}_{[t - F^j_{\mathcal{L}}(t), t + F^j_{\mathcal{L}}(t)]}(A) \ge j \qquad \forall j = 1, \ldots, n.$$

Hence $F^j_{\mathcal{L}}(t)$ is an approximated local counting function for $\sigma(A)$. They can be obtained as the j-th smallest eigenvalue μ of the non-negative weak problem:

$$\text{find } (\mu, u) \in [0, \infty) \times \mathcal{L} \backslash \{0\} \quad \text{such that} \quad q_t(u,v) = \mu^2 \langle u, v \rangle \qquad \forall v \in \mathcal{L}.$$

[§] Generally $\mathcal{E}_J(A) \subseteq \mathbb{1}_J(A)\mathcal{H}$, however there is no reason for these two subspaces to be equal.

4.5.2 Optimal setting for detection of the spectrum

From a numerical point of view it is inefficient to consider all the values t and hence one have to characterise the optimal one. The first idea may be to estimate local minima of $F^1_{\mathcal{L}}(t)$. This turns out to be the opposite and we now give a crucial ingredient in the formulation of the strategy proposed in [Dav98; Dav00; DP04].

To simplify various statements, we introduce some notations:

$$\mathfrak{n}_j^-(t) = \sup\{s < t : \operatorname{tr}\mathbb{1}_{(s,t]}(A) \geq j\} \quad \text{and}$$
$$\mathfrak{n}_j^+(t) = \inf\{s > t : \operatorname{tr}\mathbb{1}_{[t,s)}(A) \geq j\}.$$

Then $\mathfrak{n}_j^{\mp}(t)$ is the j-th point in $\sigma(A)$ to the left$(-)$/right$(+)$ of t counting multiplicities. Here $t \in \sigma(A)$ is allowed and neither t nor $\mathfrak{n}_1^{\mp}(t)$ have to be isolated from the rest of $\sigma(A)$.

Our strategy was based on the following result.

Proposition 4.14. *Let $t^- < t < t^+$. Then*

$$F^j_{\mathcal{L}}(t^-) \leq t - t^- \quad \Rightarrow \quad t^- - F^j_{\mathcal{L}}(t^-) \leq \mathfrak{n}_j^-(t)$$
$$F^j_{\mathcal{L}}(t^+) \leq t^+ - t \quad \Rightarrow \quad t^+ + F^j_{\mathcal{L}}(t^+) \geq \mathfrak{n}_j^+(t).$$

Moreover, let $t_1^- < t_2^- < t < t_2^+ < t_1^+$. Then

$$F^j_{\mathcal{L}}(t_i^-) \leq t - t_i^- \text{ for } i = 1,2 \quad \Rightarrow \quad t_1^- - F^j_{\mathcal{L}}(t_1^-) \leq t_2^- - F^j_{\mathcal{L}}(t_2^-) \leq \mathfrak{n}_j^-(t)$$
$$F^j_{\mathcal{L}}(t_i^+) \leq t_i^+ - t \text{ for } i = 1,2 \quad \Rightarrow \quad t_1^+ + F^j_{\mathcal{L}}(t_1^+) \geq t_2^+ + F^j_{\mathcal{L}}(t_2^+) \geq \mathfrak{n}_j^+(t).$$

When t is an eigenvalue of multiplicity m and $\mathcal{E}_t(A) \cap \mathcal{L} = \{0\}$, then for $t^- < t < t^+$.

$$F^j_{\mathcal{L}}(t^-) \leq t - t^- \quad \Rightarrow \quad t^- - F^j_{\mathcal{L}}(t^-) \leq \mathfrak{n}_{j+m}^-(t)$$
$$F^j_{\mathcal{L}}(t^+) \leq t^+ - t \quad \Rightarrow \quad t^+ + F^j_{\mathcal{L}}(t^+) \geq \mathfrak{n}_{j+m}^+(t).$$

For the rest of this presentation, we make the following

Assumption 4.5.1.

$$\mathcal{L} \cap \mathcal{E}_t(A) = \{0\}.$$

From Proposition 4.14 it follows that optimal lower bounds for $\mathfrak{n}_j^-(t)$ are achieved by finding $\hat{t}_j^- = s \leq t$, the furthest point to t, such that

$$t - s = F^j_{\mathcal{L}}(s). \tag{4.12}$$

Similarly, optimal upper bounds for $\mathfrak{n}_j^+(t)$ are found by analogous means.

But determining this optimal value as fixed point seems to be a challenging problem too. Following [DP04], we characterised the optimal parameters $t^{\pm}$ in Proposition 4.14 by means of a weak eigenvalue problem due to Zimmermann and Mertins [ZM95] : If $l_t : \mathrm{D}(A) \times \mathrm{D}(A) \longrightarrow \mathbb{C}$ is the (generally not closed) bilinear form associated to $(A - t)$,

$$l_t(u, w) = \langle (A - t)u, w \rangle \qquad \forall u, w \in \mathrm{D}(A),$$

we consider the weak eigenvalue problem

$$\begin{aligned} &\text{find } u \in \mathcal{L} \setminus \{0\} \text{ and } \tau \in \mathbb{R} \text{ such that} \\ &\tau q_t(u, v) = l_t(u, v) \qquad \forall v \in \mathcal{L}. \end{aligned} \tag{$\mathrm{Z}_t^{\mathcal{L}}$}$$

Let

$$\tau_1^-(t) \leq \ldots \leq \tau_{n^-}^-(t) < 0 \qquad \text{and} \qquad 0 < \tau_{n^+}^+(t) \leq \ldots \leq \tau_1^+(t),$$

be the negative and positive eigenvalues of $(\mathrm{Z}_t^{\mathcal{L}})$ respectively, $n^{\mp}(t)$ the number of these negative and positive eigenvalues and $u_j^{\mp}(t)$ denote eigenfunctions associated with $\tau_j^{\mp}(t)$.

The connection with the framework of [DP04] is made as follows. Let us recall the

Theorem 4.15. *[DP04, Theorem 11] Let $t \in \mathbb{R}$. The smallest eigenvalue $\tau = \tau_1^-(t)$ of ($Z_t^{\mathcal{L}}$) is negative if and only if there exists $s < t$ such that (4.12) holds true. In this case $s = t + \frac{1}{2\tau_1^-(t)}$ and*

$$F_{\mathcal{L}}^1(s) = -\frac{1}{2\tau_1^-(t)} = \frac{|u_1^-(t)|_s}{\|u_1^-(t)\|}$$

for $u = u_1^-(t) \in \mathcal{L}$ the corresponding eigenvector.

An extension to $j \neq 1$ is now found by induction.

Theorem 4.16. *Let $t \in \mathbb{R}$ and $1 \le j \le n$ be fixed. The number of negative eigenvalues $n^-(t)$ in ($Z_t^{\mathcal{L}}$) is greater than or equal to j if and only if*

$$\frac{\langle Au, u\rangle}{\langle u, u\rangle} < t \qquad \textit{for some} \quad u \in \mathcal{L} \ominus \operatorname{Span}\{u_1^-(t), \dots, u_{j-1}^-(t)\}.$$

Assuming this holds true, then $\tau = \tau_j^-(t)$ and $u = u_j^-(t)$ are solutions of ($Z_t^{\mathcal{L}}$) if and only if

$$F_{\mathcal{L}}^j\left(t + \frac{1}{2\tau_j^-(t)}\right) = -\frac{1}{2\tau_j^-(t)} = \frac{\left|u_j^-(t)\right|_{t+\frac{1}{2\tau_j^-(t)}}}{\|u_j^-(t)\|}.$$

A neat procedure for finding certified spectral bounds for A, as described in [ZM95], can now be deduced from Theorem 4.16 :

For all $t \in \mathbb{R}$ and $j \in \{1, \dots, n^{\pm}(t)\}$,

$$t + \frac{1}{\tau_j^-(t)} \le \mathfrak{n}_j^-(t) \qquad \text{and} \qquad \mathfrak{n}_j^+(t) \le t + \frac{1}{\tau_j^+(t)}.$$

4.5.3 Convergence and error estimates

If $\mathcal{L}$ captures an eigenspace of A within a certain order of precision $\mathcal{O}(\varepsilon)$ as specified below, we showed that the bounds which follow from Proposition 4.14, ore precisely (4.12), are

1. at least within $\mathcal{O}(\varepsilon)$ from the true spectral data for any $t \in \mathbb{R}$,
2. within $\mathcal{O}(\varepsilon^2)$ for $t \notin \sigma(A)$.

In the spectral approximation literature this last property is known as optimal order of convergence/exactness, see [Cha83, Chapter 6] or [Wei74].

Let us make the statement more precise. The following is one of our main results in [BBBa].

Theorem 4.17. *Let $J \subset \mathbb{R}$ be a bounded open segment such that $J \cap \sigma(A) \subseteq \sigma_{\mathrm{disc}}(A)$. Let $\{\phi_k\}_{k=1}^{\tilde m}$ be a family of eigenvectors of A such that $\operatorname{Span}\{\phi_k\}_{k=1}^{\tilde m} = \mathcal{E}_J(A)$. For fixed $t \in J$, there exist constants $\tilde\varepsilon_t > 0$ and $C_t^- > 0$ independent of the trial space $\mathcal{L}$, ensuring the following. If there are $\{w_j\}_{j=1}^{\tilde m} \subset \mathcal{L}$ such that*

$$\left(\sum_{j=1}^{\tilde m} \|w_j - \phi_j\|^2 + |w_j - \phi_j|_t^2\right)^{1/2} \le \varepsilon < \tilde\varepsilon_t, \tag{4.13}$$

then

$$0 < \nu_j^-(t) - \left(t + \frac{1}{\tau_j^-(t)}\right) \le C_t^- \varepsilon^2$$

for all $j \le n^-(t)$ such that $\nu_j^-(t) \in J$.

We also obtained a statement on convergence of eigenfunctions.

Corollary 4.18. *Let $J \subset \mathbb{R}$ be a bounded open segment such that $J \cap \sigma(A) \subseteq \sigma_{\mathrm{disc}}(A)$. Let $\{\phi_k\}_{k=1}^{\tilde{m}}$ be a family of eigenvectors of A such that* $\mathrm{Span}\{\phi_k\}_{k=1}^{\tilde{m}} = \mathcal{E}_J(A)$. *For fixed $t \in J$, there exist constants $\tilde{\varepsilon}_t > 0$ and $C_t^{\pm} > 0$ independent of the trial space $\mathcal{L}$, ensuring the following. If there are $\{w_j\}_{j=1}^{\tilde{m}} \subset \mathcal{L}$ guaranteeing the validity of (4.13), for all $j \leq n^{\pm}(t)$ such that $\nu_j^{\pm}(t) \in J$ we can find $\psi_j^{\varepsilon\pm} \in \mathcal{E}_{\{\nu_j^-(t), \nu_j^+(t)\}}(A)$ satisfying*

$$|u_j^{\pm}(t) - \psi_j^{\varepsilon\pm}|_t + \|u_j^{\pm}(t) - \psi_j^{\varepsilon\pm}\| \leq C_t^{\pm}\varepsilon.$$

Hence we achieved the optimal order of convergence. This is possible since Assumption (4.5.1) ensures that the arguments of the approximated local counting function in Theorem 4.16 are never in the spectrum.

4.5.4 The finite element method for the Maxwell eigenvalue problem

Let $\Omega \subset \mathbb{R}^3$ be a polyhedron. Denote by $\partial\Omega$ the boundary of this region and by $\mathbf{n}$ its outer normal vector. Consider the anisotropic Maxwell eigenvalue problem: find $\omega \in \mathbb{R}$ and $(\boldsymbol{E}, \boldsymbol{H}) \neq 0$ such that

$$\begin{cases} \operatorname{curl} \boldsymbol{E} = \mathrm{i}\omega\mu\boldsymbol{H} & \text{in } \Omega \\ \operatorname{curl} \boldsymbol{H} = -\mathrm{i}\omega\epsilon\boldsymbol{E} & \\ \boldsymbol{E} \times \mathbf{n} = 0 & \text{on } \partial\Omega. \end{cases} \tag{4.14}$$

The physical phenomenon of electromagnetic oscillations in a resonator is described by (4.14), assuming that the field phasor satisfies Gauß's law

$$\operatorname{div}(\epsilon\boldsymbol{E}) = 0 = \operatorname{div}(\mu\boldsymbol{H}) \quad \text{in } \Omega. \tag{4.15}$$

Here ϵ and μ, respectively, are the given electric permittivity and magnetic permeability at each point of the resonator.

The orthogonal complement in a suitable inner product, see [BS90] of the solenoidal space (4.15) is the gradient space. This gradient space has infinite dimension and is part of the kernel of the densely defined linear self-adjoint operator

$$\mathcal{M} : \mathrm{D}(\mathcal{M}) \longrightarrow L^2(\Omega)^6$$

associated to (4.14). In turns, this means that (4.14)-(4.15) and the unrestricted problem (4.14), have exactly the same non-zero spectrum and exactly the same eigenvectors orthogonal to the kernel. As already explained, the numerical computation of ω by means of the finite element method is extremely challenging, due to a combination of variational collapse ($\mathcal{M}$ is strongly indefinite) and the fact that finite element bases seldom satisfy the ansatz (4.15).

The concrete assumptions on the data of equation (4.14) were as follows. The polyhedron $\Omega \subset \mathbb{R}^3$ is open, bounded and simply connected. The permittivities are such that

$$\epsilon,\ \frac{1}{\epsilon},\ \mu,\ \frac{1}{\mu} \in L^{\infty}(\Omega).$$

Without further mention, the non-zero spectrum of $\mathcal{M}$ will be assumed to be purely discrete and it does not accumulate at $\omega = 0$. This hypothesis is verified, for example, whenever Ω is a polyhedron with a Lipschitz boundary, [Mon03, Corollary 3.49] and [BS90, Lemma 1.3]. A more systematic analysis of the spectral properties of $\mathcal{M}$ on more general regions Ω is a work in progress [BBB16].

4.5.4.1 Finite element computation of the eigenvalue bounds

Formulation of the weak problem and eigenvalue bounds. Let $\{\mathcal{T}_h\}_{h>0}$ be a family of shape-regular [EG04] triangulations of $\overline{\Omega}$, where the elements $K \in \mathcal{T}_h$ are simplexes with diameter h_K and $h = \max_{K\in\mathcal{T}_h} h_K$. For $r \geq 1$, let

$$\begin{aligned}\mathbf{V}_h^r &= \{\boldsymbol{v}_h \in C^0(\overline{\Omega})^3 : \boldsymbol{v}_h|_K \in \mathbb{P}_r(K)^3\ \forall K \in \mathcal{T}_h\}\\ \mathbf{V}_{h,0}^r &= \{\boldsymbol{v}_h \in \mathbf{V}_h^r : \boldsymbol{v}_h \times \mathbf{n} = \mathbf{0} \text{ on } \partial\Omega\}.\end{aligned}$$

Then

$$\mathcal{L} \equiv \mathcal{L}_h = \mathbf{V}_{h,0}^r \times \mathbf{V}_h^r \subset \mathcal{D}_1. \tag{4.16}$$

For $t \in \mathbb{R}$, let $\mathfrak{m}_t^p : \mathcal{D}_1 \times \mathcal{D}_1 \longrightarrow \mathbb{C}$ be given by

$$\begin{aligned}\mathfrak{m}_t^1\left(\begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{bmatrix}, \begin{bmatrix}\boldsymbol{F}\\ \boldsymbol{G}\end{bmatrix}\right) &= \int_\Omega \left((\mathcal{M}_1 - t\mathcal{P}^2)\begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{bmatrix}\right)\cdot\begin{bmatrix}\boldsymbol{F}\\ \boldsymbol{G}\end{bmatrix}\\ \mathfrak{m}_t^2\left(\begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{bmatrix}, \begin{bmatrix}\boldsymbol{F}\\ \boldsymbol{G}\end{bmatrix}\right) &= \int_\Omega \left((\mathcal{P}^{-1}\mathcal{M}_1 - t\mathcal{P})\begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{bmatrix}\right)\cdot\left((\mathcal{P}^{-1}\mathcal{M}_1 - t\mathcal{P})\begin{bmatrix}\boldsymbol{F}\\ \boldsymbol{G}\end{bmatrix}\right)\end{aligned}$$

Then $Z_t^{\mathcal{L}}$ [ZM95; DP04; BBBa] has the following form:

$$\begin{aligned}&\text{find } \left(\tau, \begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{bmatrix}\right) \in \mathbb{R} \times (\mathcal{L}\setminus\{0\}) \text{ such that}\\ &\mathfrak{m}_t^1\left(\begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{bmatrix}, \begin{bmatrix}\boldsymbol{F}\\ \boldsymbol{G}\end{bmatrix}\right) = \tau\mathfrak{m}_t^2\left(\begin{bmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{bmatrix}, \begin{bmatrix}\boldsymbol{F}\\ \boldsymbol{G}\end{bmatrix}\right) \qquad \forall \begin{bmatrix}\boldsymbol{F}\\ \boldsymbol{G}\end{bmatrix} \in \mathcal{L}.\end{aligned} \tag{4.17}$$

Let $m^\pm(t) \equiv m^\pm(t,h)$ be the number of negative and positive eigenvalues of (4.17), respectively. Let $\tau_j^\pm(t) \equiv \tau_j^\pm(t,h)$,

$$\tau_1^-(t) \leq \ldots \leq \tau^-(t)_{m^-(t)}$$

be the negative eigenvalues of (4.17) and

$$\tau_{m^+(t)}^+(t) \leq \ldots \leq \tau_1^+(t)$$

be the positive eigenvalues of (4.17), if they exist at all. Let

$$\rho_j^\pm(t,h) = t + \frac{1}{\tau_j^\pm(t)}.$$

By counting multiplicities, let

$$\ldots \leq \nu_2^-(t) \leq \nu_1^-(t) < t < \nu_1^+(t) \leq \nu_2^+(t) \leq \ldots$$

be the eigenvalues of $\mathcal{M}$ which are adjacent to t. That is $\nu_j^-(t)$ is the j-th eigenvalue strictly to the left of t and $\nu_j^+(t)$ is the j-th eigenvalue strictly to the right of t.

Convergence of the eigenvalue bounds. Consider an open bounded segment $J \subset \mathbb{R}$, such that $0 \notin J$. Denote by $\mathcal{E}_J$ the eigenspace associated to this segment and assume that $t \in J$. Here and elsewhere the relevant set where the indices j move is

$$\mathcal{F}_J^\pm(t) = \{j \in \mathbb{N} : \nu_j^\pm(t) \in J\}.$$

The following crucial statement is a direct consequence of our theoretical analysis.

Theorem 4.19. *Let $r \in \mathbb{N}$ be fixed. Then*

$$\lim_{h\to 0} \left|\rho_j^{\pm}(t,h) - \nu_j^{\pm}(t)\right| = 0 \qquad \forall j \in \mathcal{F}_J^{\pm}(t).$$

If in addition $\mathcal{P}^{-1}\mathcal{E}_J \subseteq \mathcal{H}^{r+1}(\Omega)^6$, then there exist $C_t^{\pm} \equiv C_t^{\pm}(r) > 0$ such that

$$\left|\rho_j^{\pm}(t,h) - \nu_j^{\pm}(t)\right| \le C_t^{\pm} h^{2r} \qquad \forall j \in \mathcal{F}_J^{\pm}(t)$$

for h sufficiently small.

We also obtained the convergence of the associated eigenvectors.

4.5.4.2 A certified numerical strategy

Denote by $0 < t_{\rm up} < t_{\rm low}$ the corresponding parameters t in the weak problem (4.17), which are set for computing $\rho_j^-(t_{\rm low},h)$ (lower bounds) and $\rho_j^+(t_{\rm up},h)$ (upper bounds) in the segment $(t_{\rm up},t_{\rm low})$. The scheme described next aims at finding intervals of enclosure for the eigenvalues of $\mathcal{M}$ which lie in this segment, for a prescribed tolerance set by the parameter $\delta > 0$.

Procedure 4.5.1.

Input.

- *Initial $t_{\rm up} > 0$.*
- *Initial $t_{\rm low} > t_{\rm up}$ such that $t_{\rm low} - t_{\rm up}$ is fairly large.*
- *A sub-family $\mathcal{F}$ of finite element spaces $\mathcal{L}_h$ as in (4.16), dense as $h \to 0$.*
- *A tolerance $\delta > 0$ fairly small compared with $t_{\rm low} - t_{\rm up}$.*

Output.

- *A prediction $\tilde{m}(\delta) \in \mathbb{N}$ of $\operatorname{tr}\mathbb{1}_{(t_{\rm up},t_{\rm low})}(\mathcal{M})$.*
- *Predictions $\omega_{j,\delta}^{\pm}$ of the endpoints of enclosures for the eigenvalues in $\sigma(\mathcal{M}) \cap (t_{\rm up},t_{\rm low})$, such that $0 < \omega_{j,\delta}^{+} - \omega_{j,\delta}^{-} < \delta$ for $j = 1,\dots,\tilde{m}(\delta)$.*

Steps.

1. *Set initial $\mathcal{L}_h \in \mathcal{F}$.*
2. *While*
$$\rho_{j,h}^{+} - \rho_{j,h}^{-} \ge \delta \ \text{or}\ \rho_{j,h}^{-} > \rho_{j,h}^{+} \ \text{for some}\ j = 1,\dots,\tilde{m},$$
do 3 - 5.
3. *Compute*
$$\rho_{j,h}^{+} = \rho_j^{+}(t_{\rm up},h) \qquad \text{for} \qquad j = 1,\dots,\tilde{m}_{\rm up}$$
where $\tilde{m}_{\rm up}$ is such that $\rho_{\tilde{m}_{\rm up},h}^{+} < t_{\rm low}$ and
$$\rho_{\tilde{m}_{\rm up}+1}^{+}(t_{\rm up},h) \ge t_{\rm low}.$$
4. *Compute*
$$\rho_{\tilde{m}_{\rm low}-k+1,h}^{-} = \rho_k^{-}(t_{\rm low},h) \qquad \text{for} \qquad k = 1,\dots,\tilde{m}_{\rm low}$$
where $\tilde{m}_{\rm low}$ is such that $\rho_{\tilde{m}_{\rm low},h}^{-} > t_{\rm up}$ and
$$\rho_{\tilde{m}_{\rm low}+1}^{-}(t_{\rm low},h) \le t_{\rm up}.$$

RF	DOF	$t_{\rm low} = 1.95$ $(l = 1\ \omega_3^-)$	$t_{\rm low} = 2.05$ $(l = 3\ \omega_3^-)$	$t_{\rm up} = 1.05$ $(l = 1\ \omega_3^+)$	$t_{\rm up} = 0.7$ $(l = 3\ \omega_3^+)$
1	4143	1.24764	1.26640	1.50395	1.3436
0.1	9648	1.25029	1.26830	1.49282	1.3336
0.01	74226	1.25063	1.26846	1.48899	1.3274

Figure 4.5: Dependence of the accuracy of our bounds on the choice of t for the region $\tilde{\Omega}_{\rm cut}$. It is preferable to pick $t_{\rm up}$ and $t_{\rm low}$ as far as possible from ω, than to increase the dimension of the trial subspace.

5. *If $\tilde{m}_{\rm low} \neq \tilde{m}_{\rm up}$, decrease h, set new $\mathcal{L}_h \in \mathcal{F}$ and go back to 3. Otherwise set $\tilde{m} = \tilde{m}_{\rm low} = \tilde{m}_{\rm up}$, decrease h, set new $\mathcal{L}_h \in \mathcal{F}$ and continue from 2.*
6. *Exit with $\tilde{m}(\delta) = \tilde{m}$ and $\omega^{\pm}_{j,\delta} = \rho^{\pm}_{j,h}$ for $j = 1, \ldots, \tilde{m}$.*

If the eigenfunctions of $\mathcal{M}$ lie in $\mathcal{H}^{r+1}(\Omega)^6$, then

$$\rho^+_{j,h} - \rho^-_{j,h} = O(h^{2r}).$$

This means that the exit rate of the conditional loop in Procedure 4.5.1 is also $O(h^{2r})$ as $h \to 0$.

4.5.5 Some numerical experiments

The two-dimensional Maxwell problem (2.10) exhibits all the complications concerning spectral pollution as its three-dimensional counterpart.

We denote by $\tilde{\mathcal{M}} : \tilde{\mathcal{D}} \longrightarrow L^2(\tilde{\Omega})^3$ the self-adjoint operator associated to (2.10). This operator has often been employed for tests which can then be validated against numerical calculations for the original Neumann Laplacian via the Galerkin method, [Dau04]. Note that the latter is a semi-definite operator with a compact resolvent, so it does not exhibit spectral pollution.

A non-Lipschitz domain. For a single trial space $\mathcal{L}$, the accuracy of the eigenvalue bounds we established depends on the position of t relative to adjacent components of the spectrum. In this experiment we demonstrate that this dependence might vary significantly with t. The numerical evidence, see figure 4.5, suggests that a good choice of $t_{\rm up}$ and $t_{\rm low}$ plays a major role in the design of efficient algorithms for eigenvalue calculation based on this method.

Let $\tilde{\Omega} \equiv \tilde{\Omega}_{\rm cut} = (0,\pi)^2 \setminus S$ for $S = [\pi/2, \pi] \times \{\pi/2\}$. Benchmarks [Dau04] on the eigenvalues of (2.10) are found by means of solving numerically the corresponding Neumann Laplacian problem.

The first seven positive eigenvalues are

$$\omega_1 \approx 0.647375015,\ \omega_2 = 1,\ \omega_3 \approx 1.280686161,$$
$$\omega_4 = \omega_5 = 2,\ \omega_6 \approx 2.096486081 \quad \text{and} \quad \omega_7 \approx 2.229523505.$$

The eigenfunctions associated to ω_2, ω_4 and ω_5 are smooth, as they are also eigenfunctions on $\tilde{\Omega}_{\rm sqr}$. On the other hand, ω_1 and ω_3 correspond to singular eigenfunctions. Standard nodal elements are completely unsuitable for the computation of these eigenvalues, even with a significant refinement of the mesh on S.

j	ω_j from [Dau04]	$\omega_j \, {}^{+}_{-}$	l	up	low
1	1.15954813181	1.159^{555}_{456}		1	85
2	1.16804100636	1.16^{807}_{770}		2	84
3	1.5834295853	1.5834^{453}_{229}		3	83
4	2.3757369919	2.375^{788}_{452}		4	82
5	2.4724291674	2.472^{479}_{212}		5	81
6	2.5288205712	2.528^{884}_{634}		6	80
7	2.7487894882	2.748^{868}_{693}		7	79
8	3.2334726763	3.23^{362}_{280}		8	78
9	3.47832176265	3.47^{8478}_{775}		9	77
10	3.51802898831	3.51^{822}_{718}		10	76

Figure 4.6: Enclosures for the first 10 positive eigenvalues of $\tilde{\mathcal{M}}$ for the transmission problem (Section 4.5.5). For comparison, on the second column we include the upper bounds found in [Dau04]. Here the trial subspace is made out of Lagrange elements of order 1, $t_{\text{up}} = 10^{-9}$ and $t_{\text{low}} = 11.74$. The mesh employed was constructed in an unstructured fashion in the four sub-domains $\tilde{\Omega}_{\text{sqr},l}$. The maximum element size is set to $h = .01$ and the total number of DOF=399720.

The table in Figure 4.5 shows computation of $\omega_3^{\pm}$ on a mesh that is increasingly refined at S with a factor RF for two pairs of choices of t_{up} and t_{low}. Here $h = 0.1$ and we consider Lagrange elements of order $r = 1$. The choice of t_{up} and t_{low} further from ω_3, even with the very coarse mesh, provides a sharper estimate of $\omega_3^{\pm}$ than the other choices even with a finer mesh.

The transmission problem. In this example, we considered a non-constant electric permittivity. Let

$$\Omega_{\text{sqr},1} = \left(0, \frac{\pi}{2}\right) \times \left(0, \frac{\pi}{2}\right) \qquad \Omega_{\text{sqr},2} = \left(\frac{\pi}{2}, \pi\right) \times \left(\frac{\pi}{2}, \pi\right)$$
$$\Omega_{\text{sqr},3} = \left(\frac{\pi}{2}, \pi\right) \times \left(0, \frac{\pi}{2}\right) \qquad \text{and} \qquad \Omega_{\text{sqr},4} = \left(0, \frac{\pi}{2}\right) \times \left(\frac{\pi}{2}, \pi\right).$$

so that

$$\overline{\tilde{\Omega}_{\text{sqr}}} = \overline{\bigcup_{l=1}^{4} \tilde{\Omega}_{\text{sqr},l}}.$$

Set $\mu = 1$ and

$$\epsilon(x) = \begin{cases} 1 & x \in \Omega_{\text{sqr},1} \cup \Omega_{\text{sqr},2} \\ \frac{1}{2} & x \in \Omega_{\text{sqr},3} \cup \Omega_{\text{sqr},4}. \end{cases}$$

Numerical estimations of the eigenvalues of $\tilde{\mathcal{M}}$ on $\tilde{\Omega} \equiv \tilde{\Omega}_{\text{sqr}}$ for this data were found in [Dau04].

We have set the experiment reported in Figure 4.5.5, on a family of meshes, which is unstructured but of equal maximum element sizes in each one of the subdomains $\tilde{\Omega}_{\text{sqr},l}$. We implemented Procedure 4.5.1 as discussed previously, with fixed $t_{\text{up}} = 10^{-9}$ and $t_{\text{low}} = 11.74$. For comparison, in the second column of the table we have included the benchmark upper bounds from [Dau04].

As we pointed out previously, accuracy depends on the regularity of the corresponding eigenspace. Moreover, finding conclusive lower bounds for the ninth and tenth eigenvalues turns out to be expensive, if $t_{\text{low}} \approx 3.5$. Observe that, from the reproduced values in the second column of the table, these two eigenvalues form a cluster of multiplicity 2. It seems that in fact they are part of a larger cluster. The resulting narrow gap from this cluster seems to be the cause of the deterioration in accuracy.

The data has a natural symmetry with respect to the diagonals of $\tilde{\Omega}_{\text{sqr}}$. Four types of eigenvectors arise from these symmetries, and the analytical problem reduces to four different eigen-problems which give rise to degenerate eigenspaces. As we were not considering a mesh that completely respects these symmetries, the multiplicities arising from them are not shown completely in the numerics.

In order to find reasonable bounds for ω_9 and ω_{10}, we had to resource to exploiting the fact that $\rho_j^-(t,h)$ is locally non-increasing in t, and it respects ordering in j. An analytical proof of this property is achieved by extending to the indefinite case the results of [BH13b, §3], but in the present context we have examined them only from a numerical perspective. Note that, when t_{low} is near to cross an eigenvalue, $\rho_j^-(t_{\text{low}},h)$ jumps. These jumps appear to be small (respecting the order of the j) as long as the subspace captures well the eigenvectors. This effect will disappear eventually as we increase t_{low} further, due to the fact that $\mathcal{L}$ is finite-dimensional. In our experiments, we have determined that $t = t_{\text{low}} \approx 11.74$ is near to optimal for the trial subspaces employed. Note that $t_{\text{low}} = 11.74$ gives 85 eigenvalues in the segment $(10^{-9}, 11.74)$ for these trial subspaces.

References

[AFW10] D. Arnold, R. S. Falk, and R. Winther. “ Finite element exterior calculus: from Hodge theory to numerical stability ”. In: *Bull. Amer. Math. Soc.* 47.2 (2010), pp. 281–354.

[AGM06] L. Aceto, P. Ghelardoni, and M. Marletta. “ Numerical computation of eigenvalues in spectral gaps of Sturm-Liouville operators ”. In: *J. Comput. Appl. Math.* 189.1-2 (2006), pp. 453–470.

[Atk+94] F. V. Atkinson, H. Langer, R. Mennicken, and A. A. Shkalikov. “ The essential spectrum of some matrix operators ”. In: *Math. Nachr.* 167 (1994), pp. 5–20.

[BB10] L. Boulton and N. Boussaïd. “ Non-variational computation of the eigenstates of Dirac operators with radially symmetric potentials ” . In: *LMS J. Comput. Math.* 13 (2010), pp. 10–32. DOI: 10.1112/S1461157008000429. URL: http://hal.archives-ouvertes.fr/hal-00308843/PDF/Preprint-DiracNumerical.pdf.

[BBBa] G. R. Barrenechea, L. Boulton, and N. Boussaïd. *Eigenvalue enclosures*. URL: http://hal.archives-ouvertes.fr/hal-00837475.

[BBBb] G. R. Barrenechea, L. Boulton, and N. Boussaïd. *Finite element eigenvalue enclosures for the Maxwell operator*. URL: http://hal.archives-ouvertes.fr/hal-00949589.

[BBBc] G. Barrenechea, L. Boulton, and N. Boussaïd. “ Some remarks on the spectral properties of the maxwell operator on rough domains and domains with symmetries ”.

[BBB16] G. Barrenechea, L. Boulton, and N. Boussaïd. “ Various remarks on the spectral properties of the Maxwell operator on rough domains and domains with symmetries ”. 2016.

[BBG00] D. Boffi, F. Brezzi, and L. Gastaldi. " On the problem of spurious eigenvalues in the approximation of linear elliptic problems in mixed form ". In: *Math. Comp.* 69.229 (2000), pp. 121–140.

[BBG98] D. Boffi, F. Brezzi, and L. Gastaldi. "Mixed finite elements for Maxwell's eigenproblem: the question of spurious modes". In: *ENUMATH 97 (Heidelberg)*. 1998, pp. 180–187.

[BBL12] L. Boulton, N. Boussaïd, and M. Lewin. " Generalised Weyl theorems and spectral pollution in the Galerkin method " . In: *J. Spectr. Theory* 2.4 (2012), pp. 329–354. DOI: 10.4171/JST/32. URL: http://hal.archives-ouvertes.fr/hal-00536270/PDF/Weyl32.pdf.

[Beh09] H. Behnke. " Lower and Upper Bounds for Sloshing Frequencies ". In: *Inequalities and Applications* (2009), pp. 13–22.

[Bet+13] T. Betcke, N. J. Higham, V. Mehrmann, C. Schröder, and F. Tisseur. *NLEVP: A Collection of Nonlinear Eigenvalue Problems*. Feb. 2013. DOI: 10.1145/2427023.2427024. URL: http://www.mims.manchester.ac.uk/research/numerical-analysis/nlevp.html.

[BH13a] L. Boulton and A. Hobiny. " On the convergence of the quadratic method ". In: *ArXiv e-prints* (July 2013). arXiv: 1307.0313 [math.NA].

[BH13b] L. Boulton and A. Hobiny. " On the quality of complementary bounds for eigenvalues ". In: *ArXiv e-prints* (Nov. 2013). arXiv: 1311.5181 [math.SP].

[BL07] L. Boulton and M. Levitin. " On Approximation of the Eigenvalues of Perturbed Periodic Schrodinger Operators ". In: *J. Phys. A: Math. Theor.* 40.31 (2007), pp. 9319–9329.

[BM01] H. Behnke and U. Mertins. " Bounds for eigenvalues with the use of finite elements ". In: *Perspectives on Enclosure Methods* (2001), p. 119.

[Bou07] L. Boulton. " Non-variational approximation of discrete eigenvalues of self-adjoint operators ". In: *IMA J. Numer. Anal.* 27.1 (2007), pp. 102–121.

[BS12] L. Boulton and M. Strauss. " Eigenvalue enclosures and convergence for the linearized MHD operator " . In: *BIT* 52.4 (2012), pp. 801–825. DOI: 10.1007/s10543-012-0389-x. URL: http://dx.doi.org/10.1007/s10543-012-0389-x.

[BS90] M. Birman and M. Solomyak. " The self-adjoint Maxwell operator in arbitrary domains ". In: *Leningrad Math. J* 1.1 (1990), pp. 99–115.

[CDL08] É. Cancès, A. Deleurence, and M. Lewin. " Non-perturbative embedding of local defects in crystalline materials " . In: *J. Phys.: Condens. Matter* 20 (2008), p. 294213. DOI: 10.1088/0953-8984/20/29/294213.

[Cha83] F. Chatelin. *Spectral Approximation of Linear Operators*. New York, 1983.

[Dau04] M. Dauge. *Computations for Maxwell equations for the approximation of highly singular solutions*. 2004. URL: http://perso.univ-rennes1.fr/monique.dauge/benchmax.html.

[Dav00] E. B. Davies. " A hierarchical method for obtaining eigenvalue enclosures ". In: *Math. Comp.* 69.232 (2000), pp. 1435–1455.

[Dav98] E. B. Davies. " Spectral enclosures and complex resonances for general self-adjoint operators " . In: *LMS J. Comput. Math.* 1 (1998), pp. 42–74. DOI: 10.1112/S1461157000000140. URL: http://dx.doi.org/10.1112/S1461157000000140.

[DG81] G. W. F. Drake and S. P. Goldman. " Application of discrete-basis-set methods to the Dirac equation " . In: *Phys. Rev. A* 23.5 (May 1981), pp. 2093–2098. DOI: 10.1103/PhysRevA.23.2093.

[DP04] E. B. Davies and M. Plum. " Spectral pollution ". In: *IMA J. Numer. Anal.* 24.3 (2004), pp. 417–438.

[DS02] M. Dauge and M. Suri. " Numerical approximation of the spectra of non-compact operators arising in buckling problems ". In: *J. Numer. Math.* 10.3 (2002), pp. 193–219.

[EG04] A. Ern and J.-L. Guermond. *Theory and practice of finite elements*. Vol. 159. Applied Mathematical Sciences. New York, 2004, pp. xiv+524.

[GA86] F. Goerisch and J. Albrecht. "The convergence of a new method for calculating lower bounds to eigenvalues". In: *Equadiff 6 (Brno, 1985)*. Vol. 1192. Lecture Notes in Math. Berlin, 1986, pp. 303–308.

[Gra82] I. P. Grant. " Conditions for convergence of variational solutions of Dirac's equation in a finite basis " . In: *Phys. Rev. A* 25.2 (Feb. 1982), pp. 1230–1232. DOI: 10.1103/PhysRevA.25.1230.

[KLT04] M. Kraus, M. Langer, and C. Tretter. " Variational principles and eigenvalue estimates for unbounded block operator matrices and applications ". In: *J. Comput. Appl. Math.* 171.1-2 (2004), pp. 311–334.

[Kut84] W. Kutzelnigg. " Basis set expansion of the Dirac operator without variational collapse ". In: *Int. J. Quantum Chemistry* 25 (1984), pp. 107–129.

[LS04] M. Levitin and E. Shargorodsky. " Spectral pollution and second-order relative spectra for self-adjoint operators ". In: *IMA J. Numer. Anal.* 24.3 (2004), pp. 393–416.

[LS10] M. Lewin and É. Séré. " Spectral pollution and how to avoid it (with applications to Dirac and periodic Schrödinger operators) " . In: *Proc. Lond. Math. Soc. (3)* 100.3 (2010), pp. 864–900. DOI: 10.1112/plms/pdp046. URL: http://dx.doi.org/10.1112/plms/pdp046.

[Mar10] M. Marletta. " Neumann-Dirichlet maps and analysis of spectral pollution for non-self-adjoint elliptic PDEs with real essential spectrum ". In: *IMA J. Numer. Anal.* 30.4 (2010), pp. 887–897.

[Mon03] P. Monk. *Finite element methods for Maxwell's equations*. Cambridge, 2003.

[Rap+97] J. Rappaz, J. Sanchez Hubert, E. Sanchez Palencia, and D. Vassiliev. " On spectral pollution in the finite element approximation of thin elastic "membrane" shells ". In: *Numer. Math.* 75.4 (1997), pp. 473–500.

[SH84] R. E. Stanton and S. Havriliak. " Kinetic balance: A partial solution to the problem of variational safety in Dirac calculations " . In: *J. Chem. Phys.* 81.4 (1984), pp. 1910–1918. DOI: 10.1063/1.447865. URL: http://link.aip.org/link/?JCP/81/1910/1.

[SW93] G. Stolz and J. Weidmann. " Approximation of isolated eigenvalues of ordinary differential operators ". In: *J. Reine Angew. Math.* 445 (1993), pp. 31–44.

[SW95] G. Stolz and J. Weidmann. " Approximation of isolated eigenvalues of general singular ordinary differential operators ". In: *Results Math.* 28.3-4 (1995), pp. 345–358.

[Wei74] H. F. Weinberger. *Variational methods for eigenvalue approximation.* Based on a series of lectures presented at the NSF-CBMS Regional Conference on Approximation of Eigenvalues of Differential Operators, Vanderbilt University, Nashville, Tenn., June 26–30, 1972, Conference Board of the Mathematical Sciences Regional Conference Series in Applied Mathematics, No. 15. 1974, pp. v+160.

[ZM95] S. Zimmermann and U. Mertins. " Variational bounds to eigenvalues of self-adjoint eigenvalue problems with arbitrary spectrum ". In: *Z. Anal. Anwendungen* 14.2 (1995), pp. 327–345.

III.5

Dispersive properties of Dirac type models

In this section, we present the results of [BG10; BDF11], where we considered dispersive properties of Dirac type linear equations. Both are *in fine*, propagation-type estimates in the sense that they imply the decay of the solution in some Banach subspace continuously embedded in the Hilbert space of square integrable spinors.

This kind of estimates are in general useful to establish dispersive estimates, that is estimates for translation invariant spaces such as L^p-spaces. Typical examples of dispersive estimates are the Strichartz estimates. Unfortunately such an implication is unclear when we consider long range perturbations, but is now classical for short-range ones, see [RS04, Section 4].

Our first result, [BG10], is a Kato-smoothness estimates for coulombic interactions while the second, [BDF11], is a Morawetz type estimate for magnetic perturbations. The techniques used in the proof of both estimates are based on commutators estimates. In the first case, we use Mourre estimates while in the second, we use the Morawetz multiplier method.

Introduction

The first propagation estimates we obtained are :

$$\int_{\mathbb{R}} \|\langle Q\rangle^{-1} e^{-\mathrm{i}tH_\gamma} \mathbb{1}_{\mathcal{I}}(H_\gamma) f\|^2 dt \le C' \|f\|^2,$$

where H_γ, see (2.6), is a perturbation of Dirac operator by multi-centre coulombic potentials with small coupling constant γ, $\mathbb{1}_{\mathcal{I}}(H_\gamma)$ is the spectral projector associates to the interval $\mathcal{I}$. In the present case, $\mathcal{I}$ is a small neighbourhood of the thresholds in the essential spectrum. One can notice that when $\mathcal{I}$ is a bounded interval in the interior of the spectrum such estimates hold, see [GM01], by means of usual Mourre estimates when the coupling constants are small. In the present case, we used a weak Mourre estimates to treat the thresholds. The question of high energies, namely when $\mathcal{I}$ is a vicinity of $+\infty$ or $-\infty$ can be treated as in Appendix B of Part I, where we provide an extension of the classical Mourre estimates to non compact intervals. The usual restriction to compact intervals in the Mourre theory is crucial to attain some critical regularity. Since the aim of this theory is to prove absence of singular spectrum the localisation in the spectrum is not a problem. In high energy, the conjugate operator to consider is the one proposed by [IM99]. In this reference, the weights are actually singular ($|Q|^{-1}$ instead of $\langle Q\rangle^{-1}$). We were able in the result we present to provide such singular weights but we needed to add a loss of regularity. This is still unclear if this loss is necessary.

The second estimates are

$$\sup_{R>0} \frac{1}{R} \int_{-\infty}^{+\infty} \int_{|x|\leq R} |(e^{itH_A} f)(x)|^2 dxdt \lesssim \|f\|_{L^2}^2.$$

where H_A is the perturbation of the Dirac operator by a magnetic potential A for which the magnetic field $B := \operatorname{curl} A$ has some decay. In this case we used Morawetz estimates.

In both cases, a smallness assumption was made in the sense that the potentials are bounded in some weighted space. While the spaces in the first case are simple weighted Lebesgue spaces, in the second they are the more elaborated Morrey-Campanato spaces.

One can notice that the first estimate implies the following

$$\sup_{R>0} \langle R\rangle^{-1} \int_{\mathbb{R}} \int_{|x|\leq R} |(e^{-itH_\gamma} \mathbb{1}_{\mathcal{I}}(H_\gamma) f)(x)|^2 dxdt \leq C' \|f\|^2.$$

which is similar to the Morawetz estimates with a non singular weight. We also notice that Morawetz estimates exclude discrete spectrum while Kato ones do not as they include projectors into the continuous part of the spectrum. Theoretically, larger perturbations should be allowed by Kato estimates.

One of the main strength of Morawetz estimates is the "simplicity" of their proof. This is a direct commutators method. They are based on the estimates of two commutations coming from two derivatives on the evolution of some localised position observable usually called Morawetz multiplier. Most of the analysis then relies on a proper choice of the multiplier in order to obtain positive second commutator and to provide useful estimates. Even if this link has to be clarified, Morawetz estimates seems to be reminiscent of Putnam's theorem [Put67] and, in the case of Schrödinger operators, Lavine's theorem [Lav71]. Let us emphasise that the proof of Morawetz estimates is a direct time-dependent analysis of the dynamics. In the other hand, Kato estimates are often obtained as a corollary of a limiting absorption principle through Bochner-Fourier transform and using refined operator theory consideration. This limiting absorption principles is often obtained by means of Mourre estimates.

In the other hand, even if the origin of the idea by Éric Mourre belongs only to him, it seems to be linked to analytic dilation methods. Somehow only the first order term in the Taylor series expansion of the dilatation is kept. The generator of dilation is now called conjugate operator and can be replaced by any type of self-adjoint operator which has a positive commutator with the operator. Eventually the analyticity is no longer needed and is replaced by C^2 type assumption. All these considerations make the analysis heavier but in a sense less demanding in terms of assumptions.

5.1 Limiting absorption principle at thresholds with an electric coupling

In [BG10], we were interested in uniform estimates of the resolvent at threshold energies of the Dirac operator in the presence of a electric potential generated by n positive point charges $(z_i)_{1\leq i\leq n}$, recall (2.6) :

$$H_\gamma := D_m + \gamma V_c(Q), \text{ where } V_c := v_c \otimes \mathrm{Id}_{\mathbb{C}^N} \text{ and } v_c(x) := \sum_{k=1,\dots,n} \frac{z_i}{|x-a_i|},$$

acting on $C_c^\infty(\mathbb{R}^3\setminus\{a_i\}_{i=1,\dots,n};\mathbb{C}^N)$, with $a_i \neq a_j$ for $i \neq j$ with $\gamma \in \mathbb{R}$ the coupling constant such that, recall (2.7),

$$Z := |\gamma| \max_{i=1,\dots,n}(|z_i|) < \sqrt{3}/2.$$

This is the multi-centre case.

Before stating our theorem let us mention briefly the bibliography. There is a larger literature for non-relativistic models, e.g., $-\Delta+V$ in $L^2(\mathbb{R}^n;\mathbb{C})$. The question is intimately linked with the presence of resonances at threshold energy, [JN01; FS04; Nak94; Ric06; Yaf82]. We mention also [Bur+04] for applications to Strichartz estimates and [DS09a; DS09b] for applications to scattering theory. We refer to [BH10; Bou11] for perturbations in divergence form and to [GH08; GH09; VW10] for some more geometrical setting. We also point out some low energy results in the context of non-relativistic quantum electrodynamics, [FGS08; FGS11].

Our main result is the

Theorem 5.1. *There are $\kappa, \delta, C > 0$ such that*

$$\sup_{|\lambda|\in[m,m+\delta],\,\varepsilon>0,|\gamma|\leq\kappa} \|\langle Q\rangle^{-1}(H_\gamma-\lambda-\mathrm{i}\varepsilon)^{-1}\langle Q\rangle^{-1}\| \leq C. \tag{5.1}$$

In particular, H_γ has no eigenvalue in $\pm m$. Moreover, there is C' so that

$$\sup_{|\gamma|\leq\kappa}\int_{\mathbb{R}} \|\langle Q\rangle^{-1}e^{-\mathrm{i}tH_\gamma}\mathbb{1}_{\mathcal{I}}(H_\gamma)f\|^2 dt \leq C'\|f\|^2, \tag{5.2}$$

where $\mathcal{I} = [-m-\delta,-m]\cup[m,m+\delta]$.

Notations : Given a complex-valued function F, $F(Q)$ is the operator of multiplication by F, $P = -\mathrm{i}\nabla$ and we use the standard $\langle\cdot\rangle := (1+|\cdot|^2)^{1/2}$.

The estimate (5.1) implies (5.2), see [ABG96, §7.1.1] or [RS78, Theorem XIII.24], so our aim was to prove (5.1).

Classical Mourre estimates do not usually hold at thresholds and this is why we considered a weak form of them. This has the advantage to deal with one major difficulty that already appears in the case $n = 1$ and $z_1 \neq 0$. Indeed it is well known that there are infinitely many eigenvalues in the gap $(-m, m)$ converging to m as soon as $\gamma < 0$ (see for instance [Tha92][Section 7.4] and references therein). This indicates for instance that a Jensen-Kato method [JK79; JN01] has no chance to provide the estimate at threshold.

In our analysis, we revisited the approach of [Ric06] and make several improvements in order to treat dispersive non self-adjoint operators and to obtain estimates of the resolvent uniformly in a parameter. These improvements were needed as the Dirac operator is matrix-valued, as we considered coulombic interactions which are singular and as we were interested in both thresholds.

Our proof was a several steps reduction of the problem to the case of a second order elliptic problem which is non-self-adjoint. The latter seemed to us easier to treat than the strongly indefinite original Dirac operator.

5.1.1 Reduction of the problem

In [FS04] and in [Ric06], one takes advantage that the Virial* of the potential is negative, in order to prove the limiting absorption principle for some self-adjoint Schrödinger operators.

*In the context of non-linear PDEs, the Virial is known as the Pohozaev identity.

We could not make this hypothesis as we were also interested in the positronic threshold, i.e., we sought a result for v and $-v$, see (5.3). It is still unclear for us if one can actually deal with thresholds energy and keep the "positivity" of something close to the quantity

$$[H_\gamma, \mathrm{i}A] - cH_\gamma,$$

for some self-adjoint operator A.

To avoid this fundamental problem, we cut-off the singularities and recovered them by perturbation. Hence we considered the resolvent of the Dirac operator perturbed by an electric potential:

$$H_\gamma^{\mathrm{bd}} := D_m + \gamma V, \text{ where } V := v \otimes \mathrm{Id}_{\mathbb{C}^N} \text{ and } v \text{ \underline{bounded}}.$$

We then add a singular part to the potential by standard perturbation techniques as we considered the addition of $V_2 \in L^1_{\mathrm{loc}}(\mathbb{R}^3; \mathbb{R}^N)$ satisfying:

$$\langle Q\rangle^2 V_2(Q) \in \mathcal{B}\big(\mathscr{H}^1(\mathbb{R}^3; \mathbb{C}^N), L^2(\mathbb{R}^3; \mathbb{C}^N)\big).$$

The fact that we recover singularities by means of perturbation allows only small coupling constants.

Hence for bounded potential V, our idea was to obtain the following limiting absorption principle

$$\sup_{|\lambda|\in[m,m+\delta],\, \varepsilon>0,\, |\gamma|\le\kappa} \|\langle Q\rangle^{-1}(H_\gamma^{\mathrm{bd}} - \lambda - \mathrm{i}\varepsilon)^{-1}\langle Q\rangle^{-1}\| \le C,$$

for some $\kappa > 0$. It was enough to consider $\lambda > 0$. Since with $\alpha_5 := \alpha_1\alpha_2\alpha_3\beta$ and using the anti-commutation relation (2.1), it is known that

$$\alpha_5\,(D_m + \gamma V)\,\alpha_5^{-1} = -(D_m - \gamma V). \tag{5.3}$$

5.1.2 The non self-adjoint operator

The non self-adjoint operator appears by expanding the resolvent relatively to a upper/lower spinor decomposition:

$$\mathbb{C}^{N/2}_{\pm} := \frac{1}{2}\,(1+\beta)\,\mathbb{C}^N$$

This transfers the analysis to the one of an elliptic operator of second order. More precisely a kind of Schur's Lemma, see also [DES00; JN01], links the inverse of the Dirac operator, with the one of a second-order operator with

Lemma 5.2. *Suppose*

$$\|v\|_\infty \le m/2 \text{ and } \nabla v \in L^\infty(\mathbb{R}^3; \mathbb{R}^3).$$

Take $z \in \mathbb{C}\setminus\mathbb{R}$ such that $\Re(z) \ge 0$. Then $\Delta_{m,v,z}$ is the minimal extension of the closable operator

$$\alpha^+ \cdot P \frac{1}{m - v(Q) + z} \alpha^- \cdot P + v(Q)$$

on $C_c^\infty(\mathbb{R}^3; \mathbb{C}^{N/2}_+)$, has domain

$$\mathcal{D}_{\min}(\Delta_{m,v,z}) = D(\Delta^*_{m,v,\bar z}) = H^2(\mathbb{R}^3; \mathbb{C}^{N/2}_+)$$

and verifies $\Delta_{m,v,z} = \Delta^*_{m,v,\bar{z}}$. *The spectrum of* $\Delta_{m,v,z}$ *is contained in the lower/upper half-plane which does not contain* z *so that* $c+z$ *is always in the resolvent set of* $\Delta_{m,v,z}$ *for any* $c \in \mathbb{R}$.

Moreover in the upper/lower spinor decomposition, we have $(H_1^{\mathrm{bd}} - z)^{-1} =$

$$\begin{pmatrix} (\Delta_{m,v,z} + m - z)^{-1} & (\Delta_{m,v,z} + m - z)^{-1}\alpha^+ \cdot P \frac{1}{m - v(Q) + z} \\ \frac{1}{m - v(Q) + z}\alpha^- \cdot P(\Delta_{m,v,z} + m - z)^{-1} & \frac{1}{m - v(Q) + z}\alpha^- \cdot P(\Delta_{m,v,z} + m - z)^{-1}\alpha^+ \cdot P \frac{1}{m - v(Q) + z} - \frac{1}{m - v(Q) + z} \end{pmatrix}$$

The drawback is that this operator is non self-adjoint and depends on the spectral parameter z. We bypass this difficulty by studying the family $\{\Delta_{m,\gamma v,\xi}\}_{(\gamma,\xi)\in\mathcal{E}}$ uniformly in $\mathcal{E}$. This is exactly why we considered a non self-adjoint extension of the weak Mourre approach of [Ric06], see Appendix C. The set $\mathcal{E}$ will be $[-\kappa,\kappa] \times [0,\delta] \times (0,1]$.

5.1.3 Positive commutator estimates

We thus needed some estimate on the resolvent of $\Delta_{m,v,z}$ uniformly in the spectral parameter.

We proved that if $v \in L^\infty(\mathbb{R}^3;\mathbb{R})$ satisfies the hypotheses

(H1) $\|v\|_\infty \le m/2$ and ∇v, $Q\cdot\nabla v(Q)$, $\langle Q\rangle(Q\cdot\nabla v)^2(Q)$ are bounded.

(H2) There are $c_v \in [0,2)$ and $c'_v \ge 0$ such that

$$x\cdot(\nabla v)(x) + c_v v(x) \le \frac{c'_v}{|x|^2}, \text{ for all } x \in \mathbb{R}^3 \setminus \{0\}$$

then the hypothesis of Section C are fulfilled.

We deduced that there are $\delta, \kappa, C_{\mathrm{LAP}} > 0$ such that

$$\sup_{\Re z\ge 0,\Im z>0,(\gamma,\xi)\in\mathcal{E}} \left\| |Q|^{-1}(\Delta_{2m,\gamma v,\xi} - z)^{-1}|Q|^{-1}\right\| \le C_{\mathrm{LAP}}.$$

Application of Appendix C. Let us be more precise on the way checked the hypothesis of Appendix C.

First for

$$\mathbb{C}^+ := \{z \in \mathbb{C}, \Im z \ge 0\},$$

we introduced

$$S := \Delta_{1,0,0} = \alpha^+ \cdot P\,\alpha^- \cdot P = -\Delta_{\mathbb{R}^3} \otimes \mathrm{Id}_{\mathbb{C}_+^{N/2}} \text{ in } H^2(\mathbb{R}^3;\mathbb{C}_+^{N/2}) \simeq H^2(\mathbb{R}^3)\otimes\mathbb{C}_+^{N/2}$$

and $\mathscr{S} := \dot{H}^1(\mathbb{R}^3;\mathbb{C}_+^{N/2})$, the homogeneous Sobolev space of order 1, (the completion of $H^1(\mathbb{R}^3;\mathbb{C}_+^{N/2})$ under the norm $\|f\|_{\mathscr{S}} := \|S^{1/2}f\|^2$), we considered the strongly continuous one-parameter unitary group $\{W_t\}_{t\in\mathbb{R}}$ acting by:

$$(W_t f)(x) = e^{3t/2} f(e^t x), \text{ for all } f \in L^2(\mathbb{R}^3;\mathbb{C}_+^{N/2}).$$

This is the C_0-group of dilatation. By interpolation and duality, one gets

$$W_t\mathscr{S} \subset \mathscr{S} \text{ and } W_t\mathscr{H}^s(\mathbb{R}^3;\mathbb{C}_+^{N/2}) \subset \mathscr{H}^s(\mathbb{R}^3;\mathbb{C}_+^{N/2}), \text{ for all } s \in \mathbb{R}.$$

Its generator A in $L^2(\mathbb{R}^3;\mathbb{C}_+^{N/2})$ was our *conjugate operator*. It acts as follows:

$$\boxed{A = \frac{1}{2}(P\cdot Q + Q\cdot P)\otimes \mathrm{Id}_{\mathbb{C}_+^{N/2}} \text{ on } C_c^\infty(\mathbb{R}^3;\mathbb{C}_+^{N/2}) \simeq C_c^\infty(\mathbb{R}^3)\otimes\mathbb{C}_+^{N/2}.}$$

By the Nelson lemma, it is essentially self-adjoint.

Then we checked that for $\delta \in (0, 2m)$:

- there are $c_1, \kappa > 0$ such that

$$\begin{aligned} D(\Delta_{2m,\gamma v,\xi}) = H^2(\mathbb{R}^3;\mathbb{C}_+^{N/2}), \quad (\Delta_{2m,\gamma v,\xi})^* = \Delta_{2m,\gamma v,\bar{\xi}}, \\ [\Re(\Delta_{2m,\gamma v,\xi}), \mathrm{i}A] - c_v\Re(\Delta_{2m,\gamma v,\xi}) \geq c_1 S > 0, \\ \mp\Im(\Delta_{2m,\gamma v,\Re(\xi)\pm \mathrm{i}\Im(\xi)}) \geq 0, \quad \mp[\Im(\Delta_{2m,\gamma v,\Re(\xi)\pm\mathrm{i}\Im(\xi)}), \mathrm{i}A] \geq 0, \end{aligned}$$

  hold true in the sense of forms on $H^1(\mathbb{R}^3;\mathbb{C}_+^{N/2})$, for all $(\gamma,\xi) \in \mathcal{E}$;

- there is c and C depending on c_v, δ, κ and v, such that

$$|\langle \Delta_{2m,\gamma v,\bar{\xi}}\, f, Ag\rangle - \langle Af, \Delta_{2m,\gamma v,\xi}\, g\rangle| \leq c\|f\|\cdot\|(\Delta_{2m,\gamma v,\xi} \pm \mathrm{i})g\|,$$

  holds true, for all $f, g \in H^2(\mathbb{R}^3;\mathbb{C}^+_{N/2}) \cap D(A)$ and

$$|\langle f, [[\Delta_{2m,\gamma v,\xi}, \mathrm{i}A], \mathrm{i}A]f\rangle| \leq C\langle f, Sf\rangle.$$

  holds true for all $f \in \mathscr{H}^1(\mathbb{R}^3;\mathbb{C}_+^{N/2})$.

This was all the assumptions we needed.

5.1.3.1 An application to non-relativistic dispersive Hamiltonians

As a by-product of our method, we obtained some new results for dispersive Schrödinger operators. In the following the dissipative part V_2 of the potential term corresponds to the absorption coefficient of the laser energy by material medium in the Helmholtz model, see [Jac75] for instance.

Theorem 5.3. *Suppose that $V_1, V_2 \in L^1_{\mathrm{loc}}(\mathbb{R}^n;\mathbb{R})$ satisfy:*

(H0) V_i are Δ-operator bounded with a relative bound $a < 1$, for $i \in \{1,2\}$.

(H1) ∇V_i, $Q\cdot\nabla V_i(Q)$ are in $\mathcal{B}(H^2(\mathbb{R}^n);L^2(\mathbb{R}^n))$ and $\langle Q\rangle(Q\cdot\nabla V_i)^2(Q)$ is bounded, for $i \in \{1,2\}$.

(H2) There are $c_1 \in [0,2)$ and $c_1' \in \big[0, 4(2-c_1)/(n-2)^2\big)$ such that

$$W_{V_1}(x) := x\cdot(\nabla V_1)(x) + c_1 V_1(x) \leq \frac{c_1'}{|x|^2}, \text{ for all } x \in \mathbb{R}^n.$$

and

$$V_2(x) \geq 0 \text{ and } -c_1 x\cdot(\nabla V_2)(x) \geq 0, \text{ for all } x \in \mathbb{R}^n.$$

On $C_c^\infty(\mathbb{R}^n)$, we define $H := -\Delta + V(Q)$, where $V := V_1 + \mathrm{i}V_2$. The closure of H defines a dispersive closed operator with domain $H^2(\mathbb{R}^n)$. We keep denoting it with H. Its spectrum included in the upper half-plane. Moreover, H has no eigenvalue in $[0,\infty)$ and

$$\sup_{\lambda\in[0,\infty),\,\mu>0} \left\| |Q|^{-1}(H-\lambda+\mathrm{i}\mu)^{-1}|Q|^{-1}\right\| < \infty. \tag{5.4}$$

If $c_1 = 0$, H has no eigenvalue in $\mathbb{R}$ and (5.4) holds true for $\lambda \in \mathbb{R}$.

The quantity W_{V_1} is called the *virial* of V_1. For fixed Planck constant as here and for a compact $\mathcal{I}$ included in $(0,\infty)$, [Roy] shows some estimates of the resolvent above $\mathcal{I}$. Here we deal with the threshold 0 and with high energy estimates. On the other hand, as he avoids the threshold, he reaches some very sharp weights.

In [Roy] one makes a hypothesis on the sign of V_2 but not on the one of $x \cdot (\nabla V_2)(x)$. Note that if one supposes $c_1 = 0$, we are also in this situation.

Unlike in [Roy], we stress that V is *not* supposed to be a relatively compact perturbation of H and that the essential spectrum of H can be different of $[0,\infty)$.

5.2 Morawetz type estimates with a magnetic field

In [BDF11], we investigated the dispersive properties of the flow $u = e^{\mathrm{i}tH_A}f$ relative to the Cauchy problem

$$\mathrm{i}u_t(t,x) + H_A u(t,x) = 0, \qquad u(0,x) = f(x) \tag{5.5}$$

where $u(t,x) : \mathbb{R}\times\mathbb{R}^3 \to \mathbb{C}^4$, $f(x) : \mathbb{R}^3 \to \mathbb{C}^4$ and H_A a magnetic perturbation of the Dirac operator :

$$H_A = -\mathrm{i}\alpha\cdot\nabla_A + m\beta = D_A + m\beta$$

where

$$D_A = -\mathrm{i}\sum_{j=1}^{3}\alpha_k(\partial_k - iA^k)$$

In [BDF11], we used a multiplier method to establish some dispersive estimates. Multiplier methods in relation with weak dispersion properties have a long history, starting from Morawetz [Mor68] for the Klein-Gordon equation and [CS88], [Sjö87], [Veg88] for the Schrödinger equation. They were adapted to more general situations in [PV99], [PV08].

In order to focus on the assumptions needed for dispersive properties we avoid any discussion on the wellposedness problem by making the

Assumption 5.2.1. *the operator H_A is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)^4$, and in addition, for initial data in $C_c^\infty(\mathbb{R}^3)^4$, the flow $e^{\mathrm{i}tH_A}f$ belongs to $C(\mathbb{R}, H^{3/2})^4$.*

The density condition allows to approximate rough solutions with smoother ones, locally uniformly in time, and is verified in concrete cases. One can actually replace the Sobolev space by the the domain of $|H_A|^{3/2}$. Our virial identities are actually restricted to smooth compactly supported functions. Most of the terms extend to the domain of the operator as $C_c^\infty(\mathbb{R}^n)$ is a core of H_A and the corresponding commutators term are bounded operators. But the computations lead to a term with B_τ which is bounded from H^s to $H^{s-3/2}$ for $s \in [1/2, 1]$, in our assumptions, this is why we imposed the $H^{3/2}$ in this assumption.

Concerning our results by using multiplier methods, we were able to partially relax the smallness assumption while making more natural assumptions from the physical point of view since they are expressed in terms of the *magnetic field*

$$B = \operatorname{curl} A,$$

which is the physically relevant quantity. Actually, our assumptions were in terms of the quantities

$$B_\tau = \frac{x}{|x|} \wedge B, \qquad \text{and} \qquad \partial_r B = (\partial_r B^1, \partial_r B^2, \partial_r B^3),$$

which are, respectively, the *tangential component* and the *radial derivative* of the field B.

5.2.1 Virial identities

We considered virial identities for

$$(\mathrm{i}\partial_t - H_A)(\mathrm{i}\partial_t + H_A) = (-\partial_{tt} - H_A^2)$$

as the Dirac operator does not have a definite sign.

Thus we reduced the study to a system of wave (Klein-Gordon) equations of the form

$$u_{tt}(t,x) + Lu(t,x) = 0, \qquad L = H_A^2 \tag{5.6}$$

with $u = u(t,x) : \mathbb{R} \times \mathbb{R}^3 \to \mathbb{C}^4$.

We obtained a virial identity for solutions of a general system of wave equations like (5.6), with L being any self-adjoint operator on $L^2(\mathbb{R}^n; C^k)$. We considered virial identities in the form

$$\dot{\Theta}(t) = \Re\left([L,\phi]u, u_t\right) \tag{5.7}$$

$$\ddot{\Theta}(t) = -\frac{1}{2}\left([L,[L,\phi]]u, u\right). \tag{5.8}$$

where

$$\Theta(t) = (\phi u_t, u_t) + \Re\left((2\phi L - L\phi)\, u, u\right).$$

for any solution $u(t,x)$ of the linear wave equation (5.6) and any function $\phi : \mathbb{R}^n \to \mathbb{R}$ smooth enough.

As an application of (5.7), (5.8) we obtained

$$\begin{aligned} &2\int_{\mathbb{R}^3} \nabla_A u D^2\phi \overline{\nabla_A u} - \frac{1}{2}\int_{\mathbb{R}^3} |u|^2 \Delta^2\phi + 2\Im \int_{\mathbb{R}^3} u\phi' B_\tau \cdot \overline{\nabla_A u} + 2\int_{\mathbb{R}^3} [S\cdot(DB\nabla\phi)\,u]\cdot\overline{u} \\ &\quad = -\frac{d}{dt}\Re\left(\int_{\mathbb{R}^3} u_t(2\nabla\phi\cdot\overline{\nabla_A u} + \overline{u}\Delta\phi)\right). \end{aligned} \tag{5.9}$$

where $DB = [\partial_j B_i]_{i,j=1,3}$, $S = \frac{i}{4}\alpha \wedge \alpha$ is the spin operator, $\phi : \mathbb{R}^3 \to \mathbb{R}$ a sufficiently smooth real valued function $\nabla_A = \nabla - iA(t,x)$ and $u(t,x)$ a solution of (5.5).

The function ϕ is the multiplier that we choose as follows. Writing $r = |x|$, for any $R > 0$, we defined ϕ as follows

$$\phi_R(r) = R\phi_0\left(\frac{r}{R}\right),$$

where

$$\phi_0(x) = \int_0^{r=|x|} \phi_0'(s)\, ds,$$

and

$$\phi_0' = \phi_0'(r) = \begin{cases} M + \frac{1}{3}r, & r \le 1 \\ M + \frac{1}{2} - \frac{1}{6r^2}, & r > 1, \end{cases}$$

with M an appropriately chosen positive constant.

5.2.2 Weak dispersion for the magnetic Dirac Equation

We applied identity (5.9) to $u = e^{\mathrm{i}tH_A}f$. For $f : \mathbb{R}^3 \to \mathbb{C}$, denoted by

$$\|f\|_{L^p_r L^\infty(S_r)} := \| \sup_{|x|=r} |f| \, \|_{L^p_r} = \left(\int_0^{+\infty} (\sup_{|x|=r} |f|)^p dr \right)^{\frac{1}{p}}.$$

and by $\nabla^r_A u$ and $\nabla^\tau_A u$ we denoted, respectively, the radial and tangential components of the covariant gradient $\nabla_A = \nabla - iA(t,x)$:

$$\nabla^r_A u = \frac{x}{|x|} \cdot \nabla_A u, \qquad \nabla^\tau_A u = \nabla_A u - \frac{x}{|x|} \nabla^r_A u,$$

and we obtained the

Theorem 5.4. *Let H_A satisfy the self-adjointness assumption (A). Let $B = \operatorname{curl} A = B_1 + B_2$ with $B_2 \in L^\infty(\mathbb{R}^n)$ and introduce the quantities*

$$C_0 = \||x|^2 B_1\|_{L^\infty(\mathbb{R}^n)}, \qquad C_1 = \||x|^{\frac{3}{2}} B_\tau\|_{L^2_r L^\infty(S_r)}, \qquad C_2 = \||x|^2 \partial_r B\|_{L^1_r L^\infty(S_r)}.$$

We shall assume the smallness conditions

$$C_0 < \frac{1}{4}, \qquad C_1^2 + 3C_2 + C_1\sqrt{C_1^2 + 6C_2} \leq 1 \tag{5.10}$$

and that the L^∞ part of B is absent in the massless case:

$$m = 0 \qquad \Longrightarrow \qquad B_2 \equiv 0.$$

Then for all $f \in L^2$, the following estimate holds:

$$\sup_{R>0} \frac{1}{R} \int_{-\infty}^{+\infty} \int_{|x|\leq R} |e^{\mathrm{i}tH_A} f|^2 dx dt \lesssim \|f\|^2_{L^2}.$$

Assume moreover that the second inequality in (5.10) is strict; then for any $f \in D(H_A)$ the following estimate is true:

$$\sup_{R>0} \frac{1}{R} \int_{-\infty}^{+\infty} \int_{|x|\leq R} |\nabla_A e^{\mathrm{i}tH_A} f|^2 dx dt + \|e^{\mathrm{i}tH_A} f\|^2_{L^\infty_x L^2_t}$$
$$+ \int_{-\infty}^{+\infty} \int_{\mathbb{R}^3} \frac{|\nabla^\tau_A e^{\mathrm{i}tH_A} f|^2}{|x|} dx dt + \sup_{R>0} \frac{1}{R^2} \int_{-\infty}^{+\infty} \int_{|x|=R} |e^{\mathrm{i}tH_A} f|^2 d\sigma dt \lesssim \|H_A f\|^2_{L^2}.$$

Example 5.5. *Explicit examples of magnetic fields satisfying assumption (5.10) are of the following form*

$$\omega\left(\frac{x}{|x|}\right) \frac{x}{|x|} + \epsilon B(x),$$

where ω is a smooth function on the unit sphere, while ϵ is sufficiently small and $B : \mathbb{R}^3 \to \mathbb{R}^3$ satisfies

$$|B_\tau(x)| \leq \frac{1}{|x|^{2-\delta} + |x|^{2+\delta}}, \qquad |\partial_r B| \leq \frac{1}{|x|^{3-\delta} + |x|^{3+\delta}},$$

for some $\delta > 0$.

5.2.3 Strichartz estimates for the magnetic Dirac Equation

We then derived from the previous weak dispersive estimates the Strichartz estimates for the perturbed Dirac equation. We recall that the solution $u(t,x) = e^{itD_0}f$ of the free massless Dirac system with initial value $u(0,x) = f(x)$ satisfies

$$\|e^{itD_0}f\|_{L^p\dot{H}_q^{\frac{1}{q}-\frac{1}{p}-\frac{1}{2}}} \lesssim \|f\|_{L^2},$$

for all wave admissible (p,q)

$$\frac{2}{p}+\frac{2}{q}=\frac{2}{2}, \qquad 2 < p \leq \infty, \qquad \infty > q \geq 2$$

while in the massive case $m \neq 0$ we have

$$\|e^{itD_m}f\|_{L^pH_q^{\frac{1}{q}-\frac{1}{p}-\frac{1}{2}}} \lesssim \|f\|_{L^2},$$

for all Schrödinger admissible (p,q)

$$\frac{2}{p}+\frac{3}{q}=\frac{3}{2}, \qquad 2 \leq p \leq \infty, \qquad 6 \geq q \geq 2.$$

These can be deduced from the corresponding estimates, respectively for the Wave equation and the Klein-Gordon equation.

A perturbation approach based on the Morawetz estimates provides

Theorem 5.6. *Assume*

$$\sum_{j\in\mathbb{Z}} 2^j \sup_{|x|\sim 2^j} |A| < \infty$$

in the perturbed case we obtained exactly the same results:

$$\|e^{\mathrm{it}D_A}f\|_{L^p\dot{H}_q^{\frac{1}{q}-\frac{1}{p}-\frac{1}{2}}} \lesssim \|f\|_{L^2}$$

for all wave admissible couple (p,q), (in particular, $p \neq 2$), while in the massive case we have, for all Schrödinger admissible couple (p,q),

$$\|e^{\mathrm{it}H_A}f\|_{L^pH_q^{\frac{1}{q}-\frac{1}{p}-\frac{1}{2}}} \lesssim \|f\|_{L^2} \qquad (m \neq 0).$$

Appendices to part III

III.C

A non-self-adjoint weak Mourre theory

We present here the non self-adjoint weak Mourre theory we developed in [BG10].

For the definitions of a regularity classes with respect to a generator of a group A such as $C^k(A)$ or $C^k(A; \mathcal{K}, \mathcal{K}^*)$ we refer to [ABG96]. The class $C^1(A)$ and $C^2(A)$ actually appears in a stronger form in the second assumption of Appendix B.

We adapted ideas coming from [FS04] and [Ric06] in order to obtain a limiting absorption principle for a family of closed operators $\{H^\pm(p)\}_{p\in\mathcal{E}}$.

We asked them to have a common domain

$$\mathscr{D} := D\big(H^+(p)\big) = D\big(H^-(p)\big), \text{ for all } p \in \mathcal{E}.$$

We choose $p_0 \in \mathcal{E}$ and endow $\mathscr{D}$ with the graph norm of $H^+(p_0)$. We also asked that

$$\big(H^+(p)\big)^* = H^-(p), \text{ for all } p \in \mathcal{E}.$$

In particular, we have that $D\big((H^\pm(p))^*\big) = \mathscr{D}$. In the sequel, we drop p, when no confusion can arise.

Since $H^\pm$ are densely defined, share the same domain and are adjoint of the other, we have that $\Re(H^\pm)$ and $\Im(H^\pm)$ are closable operators on $\mathscr{D}$, indeed their adjoints are densely defined. We denote by $\Re(H^\pm)$ and by $\Im(H^\pm)$ the closure of these operators. It is possible that they are not self-adjoint, albeit there are symmetric. However, $\mathscr{D}$ is a core for them. Their domain is possibly bigger than $\mathscr{D}$. We suppose that H^+ is *dissipative*, i.e.,

$$\langle f, \Im(H^+)f\rangle \geq 0, \text{ for all } f \in \mathscr{D}.$$

This gives also that $\Im(H^-) \leq 0$. By the numerical range theorem, we inferred that $\sigma(H^\pm)$ is included in the half-plan containing $\pm$i. Take now a non-negative self-adjoint operator S, *independent* of $p \in \mathcal{E}$, with form domain $\mathscr{G} := D(S^{1/2}) \supset \mathscr{D}$. We assume that S is injective. We write $\langle f, Sf\rangle > 0$ for all $f \in \mathscr{G} \setminus \{0\}$ or simply $S > 0$. One defines $\mathscr{S}$ as the completion of $\mathscr{G}$ under the norm $\|f\|^2_{\mathscr{S}} := \langle f, Sf\rangle$. We obtain $\mathscr{G} \subset \mathscr{S}$ with dense and continuous embedding. Moreover, since $\mathscr{G} = \langle S^{1/2}\rangle^{-1}\mathscr{H}$, $\mathscr{S}$ identifies also with the completion of $\mathscr{H}$ under the norm given by $\|S^{1/2}\langle S^{1/2}\rangle^{-1} \cdot \|$. We use the Riesz Lemma to identify $\mathscr{H}$ with $\mathscr{H}^*$, its anti-dual. The adjoint space $\mathscr{S}^*$ of $\mathscr{S}$ is exactly the domain of $\langle S^{1/2}\rangle S^{-1/2}$ in $\mathscr{H} \simeq \mathscr{H}^*$. Note that S^{-1} is an isomorphism between $\mathscr{S}$ and $\mathscr{S}^*$. We get the following scale with continuous and dense embeddings:

$$\begin{array}{ccccccccccc} & & & & & & \mathscr{S}^* & & & & \\ & & & & & & \downarrow & \searrow & & & \\ \mathscr{D} & \longrightarrow & \mathscr{G} & \longrightarrow & \mathscr{H} & \simeq & \mathscr{H}^* & \longrightarrow & \mathscr{G}^* & \longrightarrow & \mathscr{D}^*. \\ & & & \searrow & \downarrow & & & & & & \\ & & & & \mathscr{S} & & & & & & \end{array}$$

To perform our analysis, we considered an external operator, the conjugate operator. Let A be a self-adjoint operator in $\mathscr{H}$. We assume $S \in C^1(A)$. Let $W_t := e^{\mathrm{i}tA}$ be the C_0-group associated to A in $\mathscr{H}$. We ask:

$$W_t\mathscr{G} \subset \mathscr{G} \text{ and } W_t\mathscr{S} \subset \mathscr{S}, \text{ for all } t \in \mathbb{R}. \tag{C.1}$$

By duality, we have W_t stabilises $\mathscr{G}^*$ and also $\mathscr{S}^*$ (but may be not $\mathscr{D}$ or $\mathscr{D}^*$). The restricted group to these spaces is also a C_0-group. We denote the generator by A with the subspace in subscript. Given $\mathscr{H}_i \subset \mathscr{H}_j$ be two of those spaces. One easily shows that $A|_{\mathscr{H}_i} \subset A|_{\mathscr{H}_j}$ and that $A|_{\mathscr{H}_j}$ is the closure of $A|_{\mathscr{H}_i}$ in $\mathscr{H}_j$. Moreover, one has

$$D(A|_{\mathscr{H}_i}) = \left\{f \in D\big(A|_{\mathscr{H}_j}\big) \cap \mathscr{H}_i \text{ such that } A|_{\mathscr{H}_j} f \in \mathscr{H}_i\right\}.$$

We now explain how to check the second hypothesis of (C.1), see also [Ric06]. We mention this result is due to [FL74] when $D(S) \subset D(A)$.

The second invariance of the domains of (C.1) follows from the first one and from

$$|\langle Sf, Af\rangle - \langle Af, Sf\rangle| \leq c\|S^{1/2}f\|^2, \text{ for all } f \in D(S) \cap D(A).$$

Let $\mathscr{K} \subset \mathscr{H}$ be a space which is stabilised by W_t. Consider $L \in \mathcal{B}(\mathscr{K}, \mathscr{K}^*)$. We say that $L \in C^k(A; \mathscr{K}, \mathscr{K}^*)$, when $t \to W_{-t}LW_t$ is strongly C^k from $\mathscr{K}$ into $\mathscr{K}^*$. When $\mathscr{K} = \mathscr{H}$, using the resolvent equality, one observes that this class is the same as $C^k(A)$, see for instance [ABG96][Theorem 6.3.4 a.].

Theorem C.1. *Let $H^\pm = H^\pm(p)$, with $p \in \mathcal{E}$ as above. Let A be self-adjoint such that (C.1) holds true. Suppose that $H^\pm \in C^2(A; \mathscr{G}, \mathscr{G}^*)$ and that there is a constant c, independent of p, such that*

$$|\langle H^\mp f, Ag\rangle - \langle Af, H^\pm g\rangle| \leq c\|f\| \cdot \|(H^\pm \pm \mathrm{i})g\|, \text{ for all } f, g \in \mathscr{D} \cap D(A).$$

Take $c_1 \geq 0$ independent of p and assume that

$$[\Re(H^\pm), \mathrm{i}A] - c_1\Re(H^\pm) \geq S > 0,$$
$$\pm c_1[\Im(H^\pm), \mathrm{i}A] \geq 0, \quad \pm\Im(H^\pm) \geq 0,$$

in the sense of forms on $\mathscr{G}$. Suppose also there exists $C > 0$ independent of $p \in \mathcal{E}$ such that

$$\big|\langle f, \big[[H^\pm, A], A\big] f\rangle\big| \leq C\|S^{1/2}f\|^2, \text{ for all } f \in \mathscr{G}.$$

Then, there are c and $\mu_0 > 0$, both independent of p, such that

$$|\langle f, (H^\pm - \lambda \pm \mathrm{i}\mu)^{-1} f\rangle| \leq c\left(\|S^{-1/2}f\|^2 + \|S^{-1/2}Af\|^2\right) \leq c\|f\|_{D(A|_{\mathscr{S}^*})},$$

for all $p \in \mathcal{E}$, $\mu \in (0, \mu_0)$ and $\lambda \geq 0$, in the case $c_1 > 0$ and $\lambda \in \mathbb{R}$ if $c_1 = 0$.

In the self-adjoint setting, the case $c_1 = 0$ is treated in [BKM96; BM97]. Comparing with [Ric06], who deal with the case of one self-adjoint operator and for $c_1 > 0$, we gave some improvements. First, we did not ask $\mathscr{D}$ to be the domain of S. Moreover, we drop the hypothesis that the first commutator $[H, \mathrm{i}A]$ is bounded from below. For the latter, we used more carefully the numerical range theorem in our proof. But, unlike [Ric06], we did not go into interpolation theory so as to improve the norm in the limiting absorption principle. Indeed, in the context of the model we were considering here, we reached the weights we were interested in without it. We stuck to an intermediate and explicit result, which is closer to [IM99].

We mention that there exists other Mourre-like theory for non-self-adjoint operators, [Ast+06; Roy].

References

[ABG96] W. O. Amrein, A. Boutet de Monvel, and V. Georgescu. *C_0-groups, commutator methods and spectral theory of N-body Hamiltonians*. Vol. 135. Progress in Mathematics. Basel, 1996, pp. xiv+460.

[Ast+06] M. Astaburuaga, O. Bourget, V. Cortés, and C. Fernández. " Floquet operators without singular continuous spectrum. " In: *J. Funct. Anal.* 238.2 (2006), pp. 489–517. DOI: 10.1016/j.jfa.2006.03.028.

[BDF11] N. Boussaïd, P. D'Ancona, and L. Fanelli. " Virial identity and weak dispersion for the magnetic Dirac equation " . In: *J. Math. Pures Appl. (9)* 95.2 (2011), pp. 137–150. DOI: 10.1016/j.matpur.2010.10.004. URL: http://hal.archives-ouvertes.fr/hal-00430346/PDF/diracsmoo-20091218.pdf.

[BG10] N. Boussaïd and S. Golénia. " Limiting absorption principle for some long range perturbations of Dirac systems at threshold energies " . In: *Comm. Math. Phys.* 299.3 (2010), pp. 677–708. DOI: 10.1007/s00220-010-1099-3. URL: http://hal.archives-ouvertes.fr/hal-00392422/PDF/LAPDLRvHAL20090608.pdf.

[BH10] J.-F. Bony and D. Häfner. " Low frequency resolvent estimates for long range perturbations of the Euclidean Laplacian " . In: *Math. Res. Lett.* 17.2 (2010), pp. 303–308. DOI: 10.4310/MRL.2010.v17.n2.a9. URL: http://dx.doi.org/10.4310/MRL.2010.v17.n2.a9.

[BKM96] A. Boutet de Monvel, G. Kazantseva, and M. Mantoiu. " Some anisotropic Schrödinger operators without singular spectrum ". In: *Helv. Phys. Acta* 69.1 (1996), pp. 13–25.

[BM97] A. Boutet de Monvel and M. Măntoiu. *The method of the weakly conjugate operator.* Apagyi, Barnabás (ed.) et al., Inverse and algebraic quantum scattering theory. Proceedings of a conference, held at Lake Balaton, Hungary. 3–7 September 1996. Berlin: Springer. Lect. Notes Phys. 488, 204-226 (1997). 1997.

[Bou11] J.-M. Bouclet. " Low frequency estimates for long range perturbations in divergence form " . In: *Canad. J. Math.* 63.5 (2011), pp. 961–991. DOI: 10.4153/CJM-2011-022-9. URL: http://dx.doi.org/10.4153/CJM-2011-022-9.

[Bur+04] N. Burq, F. Planchon, J. G. Stalker, and A. S. Tahvildar-Zadeh. " Strichartz estimates for the wave and Schrödinger equations with potentials of critical decay " . In: *Indiana Univ. Math. J.* 53.6 (2004), pp. 1665–1680. DOI: 10.1512/iumj.2004.53.2541. URL: http://dx.doi.org/10.1512/iumj.2004.53.2541.

[CS88] P. Constantin and J.-C. Saut. " Local smoothing properties of dispersive equations " . In: *J. Amer. Math. Soc.* 1.2 (1988), pp. 413–439. DOI: 10.2307/1990923. URL: http://dx.doi.org/10.2307/1990923.

[DES00] J. Dolbeault, M. J. Esteban, and E. Séré. " On the eigenvalues of operators with gaps. Application to Dirac operators " . In: *J. Funct. Anal.* 174.1 (2000), pp. 208–226. DOI: 10.1006/jfan.1999.3542. URL: http://dx.doi.org/10.1006/jfan.1999.3542.

[DS09a] J. Dereziński and E. Skibsted. " Quantum scattering at low energies " . In: *J. Funct. Anal.* 257.6 (2009), pp. 1828–1920. DOI: 10.1016/j.jfa.2009.05.026. URL: http://dx.doi.org/10.1016/j.jfa.2009.05.026.

[DS09b] J. Dereziński and E. Skibsted. " Scattering at zero energy for attractive homogeneous potentials " . In: *Ann. Henri Poincaré* 10.3 (2009), pp. 549–571. DOI: 10.1007/s00023-009-0408-x. URL: http://dx.doi.org/10.1007/s00023-009-0408-x.

[FGS08] J. Fröhlich, M. Griesemer, and I. M. Sigal. " Spectral theory for the standard model of non-relativistic QED " . In: *Comm. Math. Phys.* 283.3 (2008), pp. 613–646. DOI: 10.1007/s00220-008-0506-5. URL: http://dx.doi.org/10.1007/s00220-008-0506-5.

[FGS11] J. Fröhlich, M. Griesemer, and I. M. Sigal. " Spectral renormalization group and local decay in the standard model of non-relativistic quantum electrodynamics " . In: *Rev. Math. Phys.* 23.2 (2011), pp. 179–209. DOI: 10.1142/S0129055X11004266. URL: http://dx.doi.org/10.1142/S0129055X11004266.

[FL74] W. G. Faris and R. B. Lavine. " Commutators and self-adjointness of Hamiltonian operators ". In: *Comm. Math. Phys.* 35 (1974), pp. 39–48.

[FS04] S. Fournais and E. Skibsted. " Zero energy asymptotics of the resolvent for a class of slowly decaying potentials ". In: *Math. Z.* 248.3 (2004), pp. 593–633.

[GH08] C. Guillarmou and A. Hassell. " Resolvent at low energy and Riesz transform for Schrödinger operators on asymptotically conic manifolds. I " . In: *Math. Ann.* 341.4 (2008), pp. 859–896. DOI: 10.1007/s00208-008-0216-5. URL: http://dx.doi.org/10.1007/s00208-008-0216-5.

[GH09] C. Guillarmou and A. Hassell. " Resolvent at low energy and Riesz transform for Schrödinger operators on asymptotically conic manifolds. II ". In: *Ann. Inst. Fourier (Grenoble)* 59.4 (2009), pp. 1553–1610. URL: http://aif.cedram.org/item?id=AIF_2009__59_4_1553_0.

[GM01] V. Georgescu and M. Măntoiu. " On the spectral theory of singular Dirac type Hamiltonians ". In: *J. Operator Theory* 46.2 (2001), pp. 289–321.

[IM99] A. Iftimovici and M. Măntoiu. " Limiting absorption principle at critical values for the Dirac operator ". In: *Lett. Math. Phys.* 49.3 (1999), pp. 235–243.

[Jac75] J. D. Jackson. *Classical electrodynamics*. Second. 1975, pp. xxii+848.

[JK79] A. Jensen and T. Kato. " Spectral properties of Schrödinger operators and time-decay of the wave functions ". In: *Duke Math. J.* 46.3 (1979), pp. 583–611.

[JN01] A. Jensen and G. Nenciu. " A unified approach to resolvent expansions at thresholds ". In: *Rev. Math. Phys.* 13.6 (2001), pp. 717–754.

[Lav71] R. B. Lavine. " Commutators and scattering theory. I. Repulsive interactions ". In: *Comm. Math. Phys.* 20 (1971), pp. 301–323.

[Mor68] C. S. Morawetz. " Time decay for the nonlinear Klein-Gordon equations ". In: *Proc. Roy. Soc. Ser. A* 306 (1968), pp. 291–296.

[Nak94] S. Nakamura. " Low energy asymptotics for Schrödinger operators with slowly decreasing potentials ". In: *Comm. Math. Phys.* 161.1 (1994), pp. 63–76. URL: http://projecteuclid.org/euclid.cmp/1104269792.

[Put67] C. R. Putnam. *Commutation properties of Hilbert space operators and related topics*. Ergebnisse der Mathematik und ihrer Grenzgebiete, Band 36. 1967, pp. xi+167.

[PV08] B. Perthame and L. Vega. “ Energy concentration and Sommerfeld condition for Helmholtz equation with variable index at infinity ” . In: *Geom. Funct. Anal.* 17.5 (2008), pp. 1685–1707. DOI: 10.1007/s00039-007-0635-6. URL: http://dx.doi.org/10.1007/s00039-007-0635-6.

[PV99] B. Perthame and L. Vega. “ Morrey-Campanato estimates for Helmholtz equations ” . In: *J. Funct. Anal.* 164.2 (1999), pp. 340–355. DOI: 10.1006/jfan.1999.3391. URL: http://dx.doi.org/10.1006/jfan.1999.3391.

[Ric06] S. Richard. “ Some improvements in the method of the weakly conjugate operator ”. In: *Lett. Math. Phys.* 76.1 (2006), pp. 27–36.

[Roy] J. Royer. “ Limiting absorption principle for the dissipative Helmholtz equation ”. URL: http://hal.archives-ouvertes.fr/hal-00380641/en/.

[RS04] I. Rodnianski and W. Schlag. “ Time decay for solutions of Schrödinger equations with rough and time-dependent potentials ” . In: *Invent. Math.* 155.3 (2004), pp. 451–513. DOI: 10.1007/s00222-003-0325-4. URL: http://dx.doi.org/10.1007/s00222-003-0325-4.

[RS78] M. Reed and B. Simon. *Methods of modern mathematical physics. IV. Analysis of operators*. New York, 1978, pp. xv+396.

[Sjö87] P. Sjölin. “ Regularity of solutions to the Schrödinger equation ” . In: *Duke Math. J.* 55.3 (1987), pp. 699–715. DOI: 10.1215/S0012-7094-87-05535-9. URL: http://dx.doi.org/10.1215/S0012-7094-87-05535-9.

[Tha92] B. Thaller. *The Dirac equation*. Texts and Monographs in Physics. Berlin, 1992, pp. xviii+357. DOI: 10.1007/978-3-662-02753-0. URL: http://dx.doi.org/10.1007/978-3-662-02753-0.

[Veg88] L. Vega. “ Schrödinger equations: pointwise convergence to the initial data ” . In: *Proc. Amer. Math. Soc.* 102.4 (1988), pp. 874–878. DOI: 10.2307/2047326. URL: http://dx.doi.org/10.2307/2047326.

[VW10] A. Vasy and J. Wunsch. “ Positive commutators at the bottom of the spectrum ” . In: *J. Funct. Anal.* 259.2 (2010), pp. 503–523. DOI: 10.1016/j.jfa.2010.04.012. URL: http://dx.doi.org/10.1016/j.jfa.2010.04.012.

[Yaf82] D. R. Yafaev. “ The low energy scattering for slowly decreasing potentials ”. In: *Comm. Math. Phys.* 85.2 (1982), pp. 177–196. URL: http://projecteuclid.org/euclid.cmp/1103921410.

III.6

Bilinear control of infinite dimensional models

In this chapter, we present the results of the analysis [BCC13c; BCC14c; BCC14a] and the short notes (proceedings) [BCC12a; BCC12b; BCC12c; BCC12e; BCC12d; BCC12a; BCC13a; BCC13b; BCC14b]. All these works were in collaboration with Marco Caponigro and Thomas Chambrion.

Our key notion of "weak coupling" was introduced in [BCC13c], where we showed many different implications. An important achievement of this series is the analysis [BCC14c]. Between this two analysis, we made a series of simple but crucial observations on the class of weakly coupled systems. All of them lead to original results and were the content of different proceedings. With two exceptions, the analysis [BCC14a] is a development of the proceeding [BCC12a] and [BCC14b] is an announcement of [BCC14c].

Introduction

These analysis are related to bilinear control of quantum systems. The general form of the problems concerns the equation

$$\frac{d}{dt}\psi(t) = A\psi(t) + u(t)B\psi(t), \tag{6.1}$$

with a given initial condition ψ_0 in some separable Hilbert space $\mathcal{H}$. The aim was to establish properties of the solution (the notion of solution has to be clarified) with respect to the time dependent coupling constant u appearing in the equation.

In general, A and B are skew-symmetric that is symmetric up to a multiplication by i. A minimal assumption in this context is that $A + u(t)B$ is skew-adjoint on the domain of A for a set of values of $u(t)$ including 0 (change of domain can be considered but introduced further complications, see for instance [Kat70]). The first question to be asked is obviously the one of well-posedness of (6.1). This turns out to be linked to the variations of u, for instance if u is a step function (piecewise constant in the following) an immediate solution is obtained by concatenating the solutions in the intervals where u is constant, see (6.4) below. This is the point of view adopted in [Cha+09; Bos+12].

We were mainly interested in the regularity of the solution both with respect to changes in u and in the scale of A. When A is a differential operator this corresponds to a Sobolev scale.

The notion of weak coupling measures at the linear level, the maximal amount of regularity than can be propagated along the flow of (6.1). As the considered regularity is in the scale associated to A, this amount is limited by the operator B. Somehow, the less changes are induced by B in the operator A the more the regularity is preserved. If A has a pure discrete spectrum this measures the strength of the couplings that B introduces between the different energy levels of A. Hence the weaker are these couplings the higher is the amount of regularity propagated by the flow associated with (6.1).

Then the question of the existence of solutions for a large class of functions u, even when B is an unbounded operator, have been considered in [BCC14c]. For instance, when u has bounded variation this is a consequence of the work by Kato [Kat53]. Under some additional assumptions on B and A, we extended his result to Radon measure, in which case we had to be careful in the notion of solution we consider. We proved using all the estimates at hand some continuity in terms of the control u. Taking advantage of Helly's selection theorem, we generalised the result on the obstruction to exact controllability by Ball, Marsden and Slemrod [BMS82], either for a larger class of control or a larger class of potentials. This analysis tells somehow that the exact controllability is an accident of regularity in the sense that the result obtained by [Bea05; BL10] are due to the strength of the control potentials that breaks the propagation of the regularity of A at some level.

Once again the starting point of these analysis, was the need to understand the properties of solutions of (6.1). Even if does not really enter the framework of our analysis its worth keeping in mind the following case $\mathcal{H} = H^s_x(\mathbb{R})$, $A = 0$, $B = x$ then the solution of (6.1) with initial condition ψ_0 is given by

$$\psi(t, x) = e^{\int_0^t u(s)\, ds x} \psi_0$$

whenever u is locally integrable. The absolute continuous function $t \mapsto \int_0^t u(s)\, ds$ can be replaced by a bounded variation function (so u can be replaced by a Radon measure) chosen to be right-continuous to comply with the initial condition requirement. In this example the growth of the norm is related to the variation of the ante-derivative of u.

6.1 A brief bibliography

The typical example we had in mind is a closed system submitted to excitations by p external fields (*e.g.* lasers) described by the bilinear Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = -\frac{1}{2}\Delta\psi + V(x)\psi(x,t) + \sum_{l=1}^{p} u_l(t) W_l(x)\psi(x,t), \tag{6.2}$$

where Δ is the Laplace-Beltrami operator on a riemanian manifold Ω, $V : \Omega \to \mathbb{R}$ is a real function, called potential, carrying the physical properties of the uncontrolled system, $W_l : \Omega \to \mathbb{R}$, $1 \leq l \leq p$, is a real function modelling the effect an external field, such as a laser, and u_l, $1 \leq l \leq p$, called control, is a real function of the time modulating the amplitude of the corresponding control potential.

In recent years there has been an increasing interest in studying the controllability of the bilinear Schrödinger equation (6.2) mainly due to its importance for many advanced applications such as Nuclear Magnetic Resonance, laser spectroscopy, and quantum information science. The problem concerns the existence of control laws $(u_1, \dots, u_p)$ steering the system from a given initial state to a pre-assigned final state in a given time. Considerable efforts have been made to study this problem and the main difficulty is the fact that the state space, namely $L^2(\Omega, \mathbb{C})$, has infinite dimension. Indeed in [BMS82], a result which implies (see [Tur00]) strong limitations on the exact controllability of the bilinear Schrödinger equation has been proved. Hence, one has to look for weaker controllability properties as, for instance, approximate controllability or controllability between eigenstates of the Schrödinger operator (which are the most relevant cases from the physical viewpoint). In dimension one, in the case $p = 1$, and for a specific class of control potentials a description of the reachable set has been provided [Bea05; BL10]. In dimension larger than one or in more general situations, the exact description of the reachable set appears to be more difficult and at the moment only approximate controllability results are available (see for example [Ner09; Cha+09; Bos+12] and references therein).

6.2 Helly's selection theorem

Before stating our result, it may be convenient to recall the definition of bounded variation function and a results that played a crucial role in our analysis: Helly's selection theorem.

Let $I \subset \mathbb{R}$ be an interval. A family $t \in I \mapsto u(t) \in E$, E a subset of a Banach space B, is in $BV(I, E)$ if there exists $N \geq 0$ such that

$$\sum_{j=1}^{n} \|u(t_j) - u(t_{j-1})\|_B \leq N$$

for any partition $a = t_0 < t_1 < \ldots < t_n = b$ of the interval (a, b). The mapping

$$u \in BV(I, E) \mapsto \sup_{a=t_0<t_1<\ldots<t_n=b} \sum_{j=1}^{n} \|u(t_j) - u(t_{j-1})\|_B$$

is a semi-norm on $BV(I, E)$ that we denote with $\|\cdot\|_{BV(I,E)}$. The semi-norm in $BV(I, E)$ is also called total variation.
We say that $(u_n)_{n\in\mathbb{N}} \in BV(I, E)$ converges to $u \in BV(I, E)$ if $(u_n)_{n\in N}$ is a bounded sequence in $BV(I, E)$ pointwise convergent to $u \in BV(I, E)$.

The Jordan decomposition theorem provides that any bounded variation function is the difference of two nondecreasing bounded functions. This coupled to Helly's principle of choice (see [Nat55]) provides the famous Helly's selection theorem :

Theorem 6.1. *Let $(f_n)_{n\in\mathbb{N}}$ be a sequence in $BV(I, \mathbb{R})$, where I is a compact interval. If*

1. *there exists $M > 0$ such that for all $n \in \mathbb{N}$, $\|f_n\|_{BV(I,\mathbb{R})} < M$,*
2. *there exists $x_0 \in I$ such that $(f_n(x_0))_{n\in\mathbb{N}}$ is bounded.*

Then $(f_n)_{n\in\mathbb{N}}$ has a pointwise convergent subsequence.

6.3 The weak coupling for piecewise constant control

In the analysis [BCC13c], we considered a slightly more general system than (6.1). In a separable Hilbert space $\mathcal{H}$ endowed with norm $\|\cdot\|$ and Hilbert scalar product $\langle\cdot,\cdot\rangle$, we studied the evolution problem

$$\frac{d\psi}{dt} = \left(A + \sum_{l=1}^{p} u_l B_l\right)\psi \tag{6.3}$$

where we made the

Assumption 6.3.1. *$(A, B_1, \dots, B_p)$ is a $(p+1)$-uple of linear operators such that*

1. *for every u in $\mathbb{R}^p$, $A + \sum_l u_l B_l$ is essentially skew-adjoint on the domain $D(A)$ of A and $\mathrm{i}(A + \sum_l u_l B_l)$ is bounded from below;*

2. *A (is skew-adjoint and) has purely discrete spectrum $(-\mathrm{i}\lambda_j)_{j\in\mathbb{N}}$, the sequence $(\lambda_j)_{j\in\mathbb{N}}$ is positive non-decreasing and unbounded.*

Assumption 2 was relaxed in [BCC14c]. In this first analysis it was advantageous to consider the compact resolvent case.

From Assumption 1, we deduce that for every initial state ψ_0 in $\mathcal{H}$, for every piecewise constant control $u : t \in \mathbb{R} \to \sum_{n=0}^{N} u^n \chi_{[t_n,t_{n+1})}(t) \in \mathbb{R}^p$, where $\chi_{[a,b)}(t)$ stands for the characteristic function of the interval $[a,b)$, with $0 = t_0 \leq t_1 \leq \ldots \leq t_{N+1}$ we can define the solution of (6.1) by $t \mapsto \Upsilon^u_t \psi_0$, where

$$\Upsilon^u_t = e^{(t-t_{j-1})(A+\sum_{l=1}^p u_l^{j-1} B_l)} \circ e^{(t_{j-1}-t_{j-2})(A+\sum_{l=1}^p u_l^{j-2} B_l)} \circ \cdots \circ e^{t_0(A+\sum_{l=1}^p u_l^0 B_l)}, \tag{6.4}$$

for $t \in [t_{j-1}, t_j)$, $j = 1, \dots, N$.

For every $s \geq 0$, with

$$|A|^s \psi = \sum_n |\lambda_n|^s \langle \psi, \phi_n \rangle \phi_n,$$

we define the s-norm by $\|\psi\|_s = \||A|^s\psi\|$ for every ψ in $D(|A|^s)$. We introduced the

Definition 6.2. *Let k be positive and let $(A, B_1, \dots, B_p)$ satisfy Assumption 6.3.1.1. Then $(A, B_1, \dots, B_p)$ is* k-weakly-coupled *if for every $u \in \mathbb{R}^p$, $D(|A + \sum_l u_l B_l|^{k/2}) = D(|A|^{k/2})$ and there exists a constant C such that, for every $1 \leq l \leq p$, for every ψ in $D(|A|^k)$, $|\Re\langle |A|^k\psi, B_l\psi\rangle| \leq C|\langle |A|^k\psi, \psi\rangle|$.*

The coupling constant *$c_k(A, B_1, \dots, B_p)$ of system $(A, B_1, \dots, B_p)$ of order k is the quantity*

$$\sup_{\psi\in D(|A|^k)\setminus\{0\}} \sup_{1\leq l\leq p} \frac{|\Re\langle |A|^k\psi, B_l\psi\rangle|}{|\langle |A|^k\psi, \psi\rangle|}.$$

In [BCC13c], we gave many different examples of weakly-coupled systems : the single trap ion, smooth potentials on compact manifold in the bounded case (such as the rotation of the molecule in a plane), or the quantum harmonic oscillator which, as the planar molecule, belongs to the class of tri-diagonal systems (the control potential has an infinite tri-diagonal matrix in the basis of the eigenvectors).

One of the main feature of weakly-coupled system is the bound on the growth of the s-norm given by the following

Proposition 6.3. *Let k be a positive number and let $(A, B_1, \dots, B_p)$ satisfy Assumption 6.3.1 and be k-weakly-coupled. Then, for every $\psi_0 \in D(|A|^{k/2})$, $K > 0$, $T \geq 0$, and piecewise constant function $u = (u_1, \dots, u_p)$ for which $\sum_{l=1}^p \|u_l\|_{L^1} \leq K$, one has*

$$\|\Upsilon^u_T(\psi_0)\|_{k/2} \leq e^{c_k(A,B_1,\dots,B_p)K}\|\psi_0\|_{k/2}. \tag{6.5}$$

If for instance the restriction of B_l to $D(|A|^{\frac{k}{2}})$ is bounded for the $\frac{k}{2}$-norm for every $l = 1, \dots, p$ then $(A, B_1, \dots, B_p)$ is k-weakly-coupled if for every $u \in \mathbb{R}^p$, $D(|A|^{\frac{k}{2}}) = D(|A + \sum_l u_l B_l|^{\frac{k}{2}})$.

6.3.1 Good Galerkin approximation

Our motivation to control the growth of the s-norm was practical. The idea was to approximate the infinite dimensional system by its compression to a natural finite dimensional space. For every N in $\mathbb{N}$, we define the orthogonal projection

$$\pi_N : \psi \in \mathcal{H} \mapsto \sum_{j \leq N} \langle \phi_j, \psi \rangle \phi_j \in \mathcal{H}$$

where $(\phi_j)_{j\in\mathbb{N}}$ a Hilbert basis of $\mathcal{H}$ such that $A\phi_j = -\mathrm{i}\lambda_j\phi_j$ for every j in $\mathbb{N}$. With this projection in mind we introduced the

Definition 6.4. *Let $N \in \mathbb{N}$. The* Galerkin approximation *of* (6.1) *of order N is the system in $\mathcal{H}$*

$$\dot{x} = \left(A^{(N)} + \sum_{l=1}^{p} u_l B_l^{(N)} \right) x \qquad (\Sigma_N)$$

where $A^{(N)} = \pi_N A \restriction_{\mathrm{Ran}\pi_N}$ and $B_l^{(N)} = \pi_N B_l \restriction_{\mathrm{Ran}\pi_N}$ are the compressions *of A and B_l (respectively).*

We denote by $X^u_{(N)}(t,s)$ the propagator of (Σ_N) for a p-uple of piecewise constant functions $u = (u_1, \ldots, u_p)$. We proved that on finite time intervals the associated sequence in N converges to the solution of (6.3) in the sense of the

Theorem 6.5 (Good Galerkin Approximation)**.** *Let k and s be non-negative numbers with $0 \leq s < k$. Let $(A, B_1, \ldots, B_p)$ satisfy Assumption 6.3.1 and be k-weakly-coupled. Assume that there exist $d > 0$ and $0 \leq r < k$ such that $\|B_l\psi\| \leq d\|\psi\|_{r/2}$ for every ψ in $D(|A|^{r/2})$ and l in $\{1, \ldots, p\}$. Then for every $\varepsilon > 0$, $K \geq 0$, $n \in \mathbb{N}$, and $(\psi_j)_{1\leq j\leq n}$ in $D(|A|^{k/2})^n$ there exists $N \in \mathbb{N}$ such that for every piecewise constant function $u = (u_1, \ldots, u_p)$*

$$\sum_{l=1}^{p} \|u_l\|_{L^1} < K \implies \|\Upsilon^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N\psi_j\|_{s/2} < \varepsilon,$$

for every $t \geq 0$ and $j = 1, \ldots, n$.

The proof of this theorem reduces, by interpolation with the estimates (6.5), to the case $s = 0$ which corresponds to the space $\mathcal{H}$.

In [BCC12b], we provided numerical experiments supporting this theorem in the case of the harmonic oscillator or the potential well. The control was of averaging type, see [Cha12] and chosen to exchange the moduli of the first three coordinates. The idea was to model quantum logical gates, the basic blocs of quantum circuits. In [BCC12c], we revisited the averaging procedure. The idea was to measure the quality of the chosen periodic control, to this effect we introduced a quantity called efficiency and made numerical experiments for rotations of planar molecules supporting that the efficiency is a good quantity to measure the quality of the control.

6.3.2 Approximate controllability

We applied the above theorem to control theory and actually generalised to higher regularity results on approximate controllability of [Bos+12]. Recall the

Definition 6.6. *Let (A, B) satisfy Assumption 6.3.1 and $s > 0$. The system (A, B) is approximately simultaneously controllable for the s-norm if for every $\psi_1, \ldots, \psi_n \in D(|A|^s)$, $\hat{\Upsilon} \in U(\mathcal{H})$ such that $\hat{\Upsilon}(\psi_1), \ldots, \hat{\Upsilon}(\psi_n) \in D(|A|^s)$, and $\varepsilon > 0$, there exists a piecewise constant function $u_\varepsilon : [0, T_\varepsilon] \to \mathbb{R}$ such that*

$$\|\hat{\Upsilon}\psi_j - \Upsilon^{u_\varepsilon}_{T_\varepsilon}\psi_j\|_s < \varepsilon.$$

for every $j = 1, \ldots, n$.

In order to state the approximate controllability result, we introduced some sufficient conditions with the

Definition 6.7. *Let (A, B) satisfy Assumption 6.3.1. A subset S of $\mathbb{N}^2$* couples *two levels j, l in $\mathbb{N}$, if there exists a finite sequence $\big((s_1^1, s_2^1), \ldots, (s_1^q, s_2^q)\big)$ in S such that*

(i) $s_1^1 = j$ and $s_2^q = l$;

(ii) $s_2^j = s_1^{j+1}$ for every $1 \le j \le q - 1$;

(iii) $\langle \phi_{s_1^j}, B\phi_{s_2^j} \rangle \ne 0$ for $1 \le j \le q$.

The subset S is called a connectedness chain *for (A, B) if S couples every pair of levels in $\mathbb{N}$. A connectedness chain is said to be* non-degenerate *(or sometimes* non-resonant*) if for every (s_1, s_2) in S, $|\lambda_{s_1} - \lambda_{s_2}| \ne |\lambda_{t_1} - \lambda_{t_2}|$ for every (t_1, t_2) in $\mathbb{N}^2 \setminus \{(s_1, s_2), (s_2, s_1)\}$ such that $\langle \phi_{t_2}, B\phi_{t_1} \rangle \ne 0$.*

We obtained the

Proposition 6.8. *Let k be a positive number. Let (A, B) satisfy Assumption 6.3.1, be k-weakly-coupled, and admit a non-degenerate chain of connectedness. Assume that there exist $d > 0$, $0 \le r < k$ such that $\|B\psi\| \le d\||A|^{\frac{r}{2}}\psi\|$, for every ψ in $D(|A|^{\frac{r}{2}})$. Then (A, B) is approximately simultaneously controllable for the norm $\|\cdot\|_{s/2}$ for every $s < k$.*

Notice that the harmonic oscillator, in the case we considered in [BCC13c], is weakly coupled at any order but not controllable, see [MR04] and it does not enter the framework of Proposition 6.8.

6.3.3 An application: The Schrödinger equation with a polarizability term

In [BCC12a; BCC14a], we considered the following control system

$$\frac{d}{dt}\psi = (A + u(t)B + u^2(t)C)\psi,$$

where (A, B, C, k) satisfies

Assumption 6.3.2. *k is an integer and (A, B, C) a triple of (possibly unbounded) linear operators in $\mathcal{H}$ such that*

1. *A is skew-adjoint with pure point spectrum $(-\mathrm{i}\lambda_j)_{j\in\mathbb{N}}$ with $\lambda_j \ne 0$, $\lambda_j \to \infty$;*
2. *for every (u_1, u_2) in $\mathbb{R}^2$, $A + u_1B + u_2C$ is essentially skew-adjoint with domain $D(A)$;*
3. *for every (u_1, u_2) in $\mathbb{R}^2$, $|A + u_1B + u_2C|^{k/2}$ has domain $D(|A|^{k/2})$);*

4. $\displaystyle \sup_{\psi \in D(|A|^k)\setminus\{0\}} \frac{|\Re\langle |A|^k\psi, B\psi\rangle|}{|\langle |A|^k\psi,\psi\rangle|} + \frac{|\Re\langle |A|^k\psi, C\psi\rangle|}{|\langle |A|^k\psi,\psi\rangle|} < +\infty$;

5. *there exist $d > 0$ and $0 \leq r < k$ such that $\|B\psi\| \leq d\||A|^{r/2}\psi\|$ and $\|C\psi\| \leq d\||A|^{r/2}\psi\|$ for every ψ in $D(|A|^{r/2})$.*

We are almost in the previous framework with $B_1 = B$, $B_2 = C$ and $u_1 = u$ but $u_2 = u^2 = u_1^2$. The later is thus a constraint in the choice of the second control.

At this point we tried to relax our requirements on the chain of connectedness and introduced the

Definition 6.9. *A pair (j,l) in $\mathbb{N}^2$ is a <u>weakly non-degenerate transition</u> of (A,B,C) if $|b_{jl}| + |c_{jl}| \neq 0$ and, for every m,n, $|\lambda_j - \lambda_l| = |\lambda_n - \lambda_m|$ implies $\{j,l\} = \{m,n\}$ or $|b_{mn}| + |c_{mn}| = 0$ or $\{m,n\} \cap \{j,l\} = \emptyset$.*

A pair (j,l) in $\mathbb{N}^2$ is a <u>strongly non-degenerate transition</u> of (A,B,C) if $|b_{jl}|+|c_{jl}| \neq 0$ and, for every m,n, $|\lambda_j - \lambda_l| = |\lambda_n - \lambda_m|$ implies $\{j,l\} = \{m,n\}$.

A pair (j,l) in $\mathbb{N}^2$ is a <u>non-resonant transition</u> of (A,B,C) if $|b_{jl}| + |c_{jl}| \neq 0$ and, for every m,n, $|\lambda_j - \lambda_l| = |\lambda_n - \lambda_m|$ implies $\{j,l\} = \{m,n\}$ or $|b_{mn}| + |c_{mn}| = 0$.

A subset S of $\mathbb{N}^2$ is a <u>chain of connectedness</u> of (A,B,C) if there exists α in $\mathbb{R}$ such that, for every $m,n \in \mathbb{N}$, there exists a finite sequence $s_1 = (s_1^1, s_1^2), s_2 = (s_2^1, s_2^2), \ldots, s_r = (s_r^1, s_r^2) \in S$ such that $s_1^1 = m$, $s_r^2 = n$, $s_l^2 = s_{l+1}^1$ for every $l = 1,\ldots,r-1$ and $\langle \phi_{s_l^2}, (B+\alpha C)\phi_{s_l^1}\rangle \neq 0$ for every $l = 1,\ldots,r$. A chain of connectedness S of (A,B,C) is <u>weakly non-degenerate</u> (resp. <u>strongly non-degenerate</u>, resp. <u>non-resonant</u>) if every s in S is a weakly non-degenerate (resp. strongly non-degenerate, resp. non-resonant) transition of (A,B,C).

By analyticity, for almost every α in $\mathbb{R}$, $(A, B+\alpha C, 0)$ satisfies Assumption 6.3.2 and admits a non-degenerate chain of connectedness. Thus due to Proposition 6.8, this system is approximatively controllable. This can be improved to impose controls in arbitrary intervals such as $[0,\delta]$ with $\delta > 0$. Then the routine introduced in the previous section works as fine.

A key remark was the following lemma. It can be interpreted as the number of values that a control takes can be restricted to the minimum that is 3 in general and 2 when it is non-negative.

Lemma 6.10. *Let $(A,B,0,k)$ satisfy Assumption 6.3.2 with k in $\mathbb{N}$, T be a positive number, a,b be two real numbers such that $a < 0 < b$, u^* be a piecewise constant function with support in $[0,T]$, and ψ_0 be in $\mathcal{H}$. Then, for every $\varepsilon > 0$, there exists a piecewise constant control $u_\varepsilon : [0,T_\varepsilon] \to \{a,0,b\}$ such that $\|\Upsilon^{u_\varepsilon}_{T_\varepsilon,0}(\psi_0) - \Upsilon^{u^*}_{T,0}(\psi_0)\| < \varepsilon$, and $\|u_\varepsilon\|_{L^1} \leq \|u^*\|_{L^1}$. Moreover, if u^* is positive, then u_ε may be chosen with value in $\{0,b\}$.*

So choosing $b = \alpha$ provided the

Theorem 6.11. *Assume that (A,B,C) admits a non-degenerate chain of connectedness. Then, for every $\varepsilon > 0$, for almost every $\delta > 0$, for every ψ_0, ψ_1 in the Hilbert unit sphere of $\mathcal{H}$, there exists $u_\varepsilon : [0,T_\varepsilon] \to \{0,\delta\}$ such that $\|\Upsilon^{u_\varepsilon}_{T_\varepsilon,0}\psi_0 - \psi_1\| < \varepsilon$.*

We also obtained that if $(1,2)$ is a non-degenerate transition of (A,B,C), then, for every $\varepsilon > 0$, for almost every $\delta > 0$, there exists $u_\varepsilon : [0,T_\varepsilon] \to \{0,\delta\}$ such that

$$\|u_\varepsilon\|_{L^1} \leq \frac{\pi}{|b_{12} + \delta c_{12}|} \text{ and } \|\Upsilon^{u_\varepsilon}_{T_\varepsilon,0}\phi_1 - \phi_2\| < \varepsilon.$$

Similarly, if for some $\delta > 0$, S is a weakly non degenerate chain of connectedness of $(A, B + \delta C, 0)$. Then, for every $\varepsilon > 0$ and for every p, q in $\mathbb{N}$, there exist $T_\varepsilon > 0$ and a piecewise constant function $u_\varepsilon : [0, T_\varepsilon] \to \{0, \delta\}$ such that

$$\|\Upsilon^{u_\varepsilon,(A,B,C)}_{T_\varepsilon,0}\phi_p - \phi_q\|_r < \varepsilon,$$

for every $r < k/2$. While if (p, q) is a weakly non-degenerate transition of (A, B, C) and for some $\delta > 0$, $b_{pq} + \delta c_{pq} \neq 0$ then, for every $\varepsilon > 0$ there exist $T_\varepsilon > 0$ and a piecewise constant function $u_\varepsilon : [0, T_\varepsilon] \to \{0, \delta\}$ such that

$$\|\Upsilon^{u_\varepsilon,(A,B,C)}_{T_\varepsilon,0}\phi_p - \phi_q\|_r < \varepsilon,$$

with

$$\|u_\varepsilon\|_{L^1} \leq \frac{\pi}{|b_{pq} + \delta c_{pq}|}$$

for every $r < k/2$.

In [BCC14a] we showed that the mapping $u \mapsto \Upsilon^u_{T,t_0}\psi_0$ admits a unique continuous extension (for the $\|\cdot\|_{L^1} + \|\cdot\|_{L^2}$ norm) to $L^1(\mathbb{R},\mathbb{R}) \cap L^2(\mathbb{R},\mathbb{R})$, for every fixed $T \geq 0$. This allowed us to extend all our results to this context.

6.3.4 Minimal control time

During our analysis, we realised that both the energy accumulating at infinity and the dispersion associated to the continuous spectrum allow in some cases very small control time. The idea relies on the RAGE theorem (Ruelle [Rue69], Amrein-Georgescu [AG74] & Enss [Ens78]), which is a manifestation of the dispersion of the control potential, and on averaging control to connect to states localised at high energies.

We considered the following bilinear control system

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -|\Delta|^\alpha \psi + u(t)\cos\theta\psi \quad \theta \in \Omega \tag{6.6}$$

where α is a real constant, $\Omega = \mathbb{R}/2\pi$ is the one dimensional torus, $\mathcal{H} = L^2(\Omega, \mathbb{C})$ and Δ is the Laplace-Beltrami operator on Ω.

The Hilbert space $\mathcal{H} = L^2(\Omega, \mathbb{C})$ splits in two subspaces $\mathcal{H}_e$ and $\mathcal{H}_o$, the spaces of even and odd functions of $\mathcal{H}$ respectively. The spaces $\mathcal{H}_e$ and $\mathcal{H}_o$ are stable under the dynamics of (6.6), hence no global controllability is to be expected in $\mathcal{H}$. We considered only the restriction of (6.6) to the space $\mathcal{H}_o$.

Theorem 6.12. *If $\alpha > 5/2$, then for every ψ_0, ψ_1 in the Hilbert unit sphere of $\mathcal{H}_o$, for every $\varepsilon > 0$, for every $T > 0$, there exists a piecewise constant function $u : [0, T] \to \mathbb{R}$ such that $\|\Upsilon^u_T\psi_0 - \psi_1\| < \varepsilon$.*

In other words, for (6.6), if $\alpha > 5/2$ then the minimal control time is arbitrary small. This situation is in contrast with the finite dimensional case. The question of minimal control time in the infinite dimensional setting is completely open. At this point, we mention the recent analysis [BCT14] which provides a general example of bilinear controlled system for which there exists a non zero minimal control time.

6.3.5 The energy of the control

In [BCC12e] we considered a couple (A, B) of linear operators such that

1. A is skew-adjoint and has purely discrete spectrum $(-\mathrm{i}\lambda_k)_{k\in\mathbb{N}}$ associated with the sequence $(\phi_k)_{k\in\mathbb{N}}$ of eigenvectors, the sequence $(\lambda_k)_{k\in\mathbb{N}}$ is positive non-decreasing and accumulates at $+\infty$;

2. $B : \mathcal{H} \to \mathcal{H}$ is skew-adjoint and bounded;

3. for every j, k, $\langle \phi_j, B\phi_k \rangle$ is purely imaginary.

Moreover we assumed that (A, B) admits a non-degenerate chain of connectedness. For every $r > 0$, for every j, k in $\mathbb{N}$ and $\varepsilon > 0$ we define $\mathcal{A}_r^\varepsilon(j,k)$ as the set of functions $u : [0, T_u] \to \mathbb{R}$ in $L^1([0,T_u]) \cap L^r([0,T_u])$ such that $\|\Upsilon^u_{T_u}\phi_j - \phi_k\| < \varepsilon$. We considered the quantity

$$\mathcal{C}_r(\phi_j, \phi_k) = \sup_{\varepsilon>0}\left(\inf_{u\in\mathcal{A}_r^\varepsilon(j,k)} \|u\|_{L^r(0,T_u)}\right).$$

and proved the

Proposition 6.13. *$\mathcal{C}_1$ is a distance on the set $\{\phi_j, j \in \mathbb{N}\}$. For $r > 1$, $\mathcal{C}_r$ is equal to zero on $\{(\phi_j, \phi_k), j, k \in \mathbb{N}\}$.*

Hence, among the Lebesgue spaces, the most relevant space seemed to be L^1 space. We actually showed that for the rotation of a planar molecule, we have

$$\mathcal{C}_1(\phi_1, \phi_2) = \pi.$$

where ϕ_1 and ϕ_2 are the first odd eigenstates.

We considered the L^1 norm as more relevant as it could play the role of an energy for the control u in the sense that this controls the variation of the solution. The outcome would be a lower bound for the energy u in terms of some distance between the initial and the final state. Actually this is still a rough norm compared to what we obtained.

In [BCC13a], we showed that from piecewise constant controls we can extend the existence and continuity results of solutions of (6.3) to bounded variation controls. Then in [BCC13b] we provided two examples (the rotation of the planar molecule and an non physical perturbation of the harmonic oscillator) for which we indeed have lower bounds of the distance of the initial and final state by means of the total variation.

For instance, if one considers only piecewise constant controls switching between 0 and some given positive value, then its total variation is a linear function of the number of its switches and only that. From the above discussion the conclusion is then that to drive the system from an initial state to a final states, there is a minimal number of switches.

Notice that up to a change of variable, corresponding to the interacting framework, the L^1 norm is nothing less than the total variation of the measure of density u. This interaction framework needs some regularity on the system, at least (A, B) has to be 1-weakly coupled.

6.4 Upper bounds for attainable set of bilinear control systems

In [BCC14c], we extended to a wider framework the considerations developed in our previous works. In this analysis, we considered only one control potential (see Equation (6.1)). As already mentioned the bounded variation control framework seemed to more suitable for non-autonomous dynamics. The idea was not new, it goes back to [Kat53]. In finite dimensions, Carathéodory's theorem allows locally integrable controls. This can be recovered when the control potential B is bounded as for instance in [BMS82]. Up to a change of variables, the interaction framework, we can extend the solutions to Radon measure. Of course, the associated solution is no longer continuous but we could impose right-continuity. It appeared that the discontinuities are located at the jumps at the atoms of the measure. Shall we be more careful, we would say that this extension to Radon measure has been obtained by a completion with respect to a natural topology on Radon measure.

We also relaxed the skew-adjointness framework in order to exploit fully the weak-coupling. Indeed, a couple (A, B) appears to be weakly coupled if B and $-B$ are dissipative (up to a constant) with respect to the scale of A.

Our aim was to give upper bounds for attainable set of bilinear control systems and our main result could be the

Theorem 6.14. *Let $\mathcal{H}$ be an infinite dimensional separable Hilbert space, A be a maximal dissipative operator on $\mathcal{H}$ with domain $D(A)$ and B an operator on $\mathcal{H}$ such that $B - c$ and $-B - c'$ generate contraction semi-groups leaving $D(A)$ invariant. If $A + uB$ is maximal dissipative with domain $D(A)$ for every u in $\mathbb{R}$ and if the map $t \in \mathbb{R} \mapsto e^{tB} A e^{-tB} \in L(D(A), \mathcal{H})$ is locally Lipschitz, then,*

1. *for every $T > 0$, there exists a unique continuous extension to $L^1([0, T], \mathbb{R})$ of the input-output mapping of (6.1) $u \mapsto \Upsilon^u_{T,0} \in L(\mathcal{H}, \mathcal{H})$,*

2. *for every ψ_0 in $\mathcal{H}$, the set*

$$\bigcup_{\alpha \geq 0} \bigcup_{T \geq 0} \bigcup_{u \in L^1([0,T],\mathbb{R})} \{\alpha \Upsilon^u_{t,0} \psi_0, t \in [0, T]\}$$

is a meagre set in $\mathcal{H}$ and hence has dense complement.

In the special case where the control operator B is bounded, we obtain a simplified statement similar to the one of [BMS82] and dealing with L^1 controls and answering a question by Ball, Marsden and Slemrod [BMS82, Remark 3.8]. We have the

Proposition 6.15. *Let $\mathcal{H}$ be an infinite dimensional separable Hilbert space, A generate a C^0 semi-group of bounded linear operators on $\mathcal{H}$ and B be a bounded linear operator on $\mathcal{H}$. Then for every $T > 0$, there exists a unique continuous extension to $L^1([0, T], \mathbb{R})$ of the input-output mapping of (6.1) $u \mapsto \Upsilon^u_{T,0} \in L(\mathcal{H}, \mathcal{H})$ and, for every ψ_0 in $\mathcal{H}$,*

$$\bigcup_{\alpha \geq 0} \bigcup_{T \geq 0} \bigcup_{u \in L^1([0,T],\mathbb{R})} \{\alpha \Upsilon^u_{t,0} \psi_0, t \in [0, T]\}$$

is a meagre set in $\mathcal{H}$ and hence has dense complement.

The Lipschitz hypothesis in Theorem 6.14 is crucial for our analysis when B is unbounded but may be difficult to check in practice. For bilinear systems encountered in quantum physics, one can take advantage of the skew-adjointness of the operators to make the analysis simpler. For instance, it is possible to replace the Lipschitz assumption of Theorem 6.14 by a hypothesis of boundedness of the commutator of operators A and B:

Theorem 6.16. *Let $\mathcal{H}$ be an infinite dimensional separable Hilbert space, k a positive number, A and B be two skew-adjoint operators such that*

1. *A is invertible,*

2. *B is A-bounded*[*] *with* $\|B\|_A = 0$, *where*

$$\|B\|_A := \inf_{\lambda>0} \|B(\lambda - A)^{-1}\|.$$

3. *for every u in* $\mathbb{R}$, $|A + uB|^{k/2}$ *is self-adjoint with domain* $D(|A|^{k/2})$ *and*

4. *there exists a constant C such that, for every* ψ *in* $D(|A|^k)$, $|\Re\langle |A|^k\psi, B\psi\rangle| \leq C|\langle |A|^k\psi, \psi\rangle|$.

Then, for every $T > 0$, *there exists a unique continuous extension to* $BV([0,T],\mathbb{R})$ *of the input-output mapping* $u \mapsto \Upsilon^u_T$. *Moreover, for every* $s < k/2$ *and every* ψ_0 *in* $\mathcal{H}$, *the set*

$$\bigcup_{\alpha\geq 0}\bigcup_{T\geq 0}\bigcup_{u\in BV([0,T],\mathbb{R})} \{\alpha \Upsilon^u_{t,0}\psi_0, t \in [0,T]\}$$

has dense complement in $D(|A|^s)$.

6.5 Some extensions

In this section, we emphasize some of the ideas behind the proofs of the above mentioned results and provide some extensions to Radon measure or higher regular framework.

6.5.1 The properties of the propagator

Under weak coupling assumption on the control potential B with respect to the uncontrolled operator A, we were able to extend the previous results to an higher regular setting.

For instance we can replace the ambient Hilbert space by any iterated domain of A up to the maximal regularity allowed by B. The immediate outcome of this extension is that the exact controllability is linked to the lack of regularity of the uncontrolled potential.

Let us recall what was our starting point. We considered as in [Kat53] the

Assumption 6.5.1. *Let I be a real interval and* $\mathcal{D}$ *dense subset of* $\mathcal{H}$

1. $A(t)$ *is a maximal dissipative operator on* $\mathcal{H}$ *with domain* $\mathcal{D}$,

2. $t \mapsto A(t)$ *has bounded variation from I to* $L(\mathcal{D},\mathcal{H})$, *where* $\mathcal{D}$ *is endowed with the graph topology associated with* $A(a)$ *for* $a = \inf I$,

3. $M := \sup_{t\in I} \|(1 - A(t))^{-1}\|_{L(\mathcal{H},\mathcal{D})} < \infty$,

Recall the

Definition 6.17 (Propagator on a Hilbert space). *Let I be a real interval. A family* $(s,t) \in \Delta_I \mapsto X(s,t)$ *of linear contractions, that is Lipschitz maps with Lipschitz constant less than one, on a Hilbert space* $\mathcal{H}$, *strongly continuous in t and s and such that*

1. *for any* $s < r < t$, $X(t,s) = X(t,r)X(r,s)$,

2. $X(t,t) = I_{\mathcal{H}}$,

is called a contraction propagator on $\mathcal{H}$.

We obtained the

[*] B is A-bounded if for instance BA^{-1} is bounded.

Theorem 6.18. *If $t \in I \mapsto A(t)$ satisfies Assumption 6.5.1, then there exists a unique contraction propagator $X : \Delta_I \to L(\mathcal{H})$ such that if $\psi_0 \in \mathcal{D}$ then $X(t,s)\psi_0 \in \mathcal{D}$ and for $(t,s) \in \Delta_I$*

$$\|A(t)X(t,s)\psi_0\| \leq Me^{M\|A\|_{BV(I,L(\mathcal{D},\mathcal{H}))}}\|A(s)\psi_0\|.$$

and in this case $X(t,s)\psi_0$ is strongly left differentiable in t and right differentiable in s with derivative (when $t = s$) $A(t+0)\psi_0$ and $-A(t-0)\psi_0$ respectively.

In the case in which $t \mapsto A(t)$ is continuous and skew-adjoint, if $\psi_0 \in \mathcal{D}$ then $t \in (s,+\infty) \mapsto X(t,s)\psi_0$ is strongly continuously differentiable in $\mathcal{H}$ with derivative $A(t)X(t,s)\psi_0$.

Below, we will write that X is the propagator associated with A. We obtained the continuity of the propagator X with respect to A in the sense of

Proposition 6.19. *Let $(A_n)_{n\in\mathbb{N}}$ and A satisfy Assumption 6.5.1 on a bounded real interval I. Let $(\mathcal{D}_n)_{n\in\mathbb{N}}$ and $\mathcal{D}$ be their respective domains (for any $t \in I$). Let X_n (respectively X) be the contraction propagator associated with A_n (respectively A).*

Assume

1. $\sup_{n\in N}\sup_{t\in I}\|(1-A_n(t))^{-1}\|_{L(\mathcal{H},\mathcal{D}_n)} < +\infty$,
2. *$A_n(\tau)$ converges to $A(\tau)$ in the strong resolvent sense for almost every $\tau \in I$ as n tends to infinity:*

$$(1-A_n(\tau))^{-1}\phi \to (1-A(\tau))^{-1}\phi \text{ in } \mathcal{H}, \text{ for a.e. } \tau \in I,$$

3. $\sup_{n\in\mathbb{N}}\|A_n\|_{BV(I,L(\mathcal{D}_n,\mathcal{H}))} < +\infty$,
4. $\sup_{n\in\mathbb{N}}\|A_n(a)\|_{L(\mathcal{D}_n,\mathcal{H}))} < +\infty$ *for for $a = \inf I$.*

Then $X_n(t,s)$ tends strongly to $X(t,s)$ locally uniformly in $s,t \in I$.

It is interesting to notice that when restated for $A_n(t) = A + u_n(t)B$ as in (6.1), the hypotheses of this proposition in the sequence $(u_n)_{n\in\mathbb{N}}$ of bounded variation functions reduces to the claim that it is almost everywhere pointwise convergent with a uniform bounded variation. This is, surprisingly, the conclusion of Helly's selection theorem and lead us to consider the corresponding topology in our analysis.

This two results provide most of the result we needed when we dealt with bounded variation controls. In the case of Radon measures we made the

Assumption 6.5.2. *(A,B,K) is a triple with A is a maximal dissipative operator on $\mathcal{H}$, B an operator on $\mathcal{H}$ with $D(A) \subset D(B)$, and K a real interval containing 0 is such that for any $u \in K$, $A + uB$ is a maximal dissipative operator on $\mathcal{H}$ with domain $D(A)$.*

We also made the

Assumption 6.5.3. *(A,B,K), with A a maximal dissipative operator on $\mathcal{H}$ and K a real interval containing 0, is such that*

1. *there exists $c \geq 0$ and $c' \geq 0$ such that $B - c$ and $-B - c'$ generate contraction semigroups on $\mathcal{H}$ leaving $D(A)$ invariant,*
2. *for every $u \in \mathcal{R}((0,T])$, with $u((0,t]) \in K$ for any $t \in [0,T]$,*

$$t \in [0,T] \mapsto \mathcal{A}(t) := e^{u((0,t])B}Ae^{-u((0,t])B}$$

is a family of maximal dissipative operators with common domain $D(A)$ such that :

- $\sup_{t\in[0,T]} \|(1-\mathcal{A}(t))^{-1}\|_{L(\mathcal{H},D(A))} < +\infty$,
- *$\mathcal{A}$ has bounded variation from $[0,T]$ to $L(D(A),\mathcal{H})$.*

This allows us to obtain the proposition below where the space $\mathcal{R}(I)$ denotes the space of (signed) Radon measures on a real interval I.

Proposition 6.20. *Let (A,B,K) satisfy Assumption 6.5.2 and (A,B,K) satisfy Assumption 6.5.3. Let $t\mapsto Y_t^u$ be the contraction propagator with initial time $s=0$ associated with $\mathcal{A}(t) := e^{-u((0,t])B}Ae^{u((0,t])B}$ for $u\in\mathcal{R}((0,T])$ and Υ_t^u the one associated with $A+u(t)B$ with initial time $s=0$ for $u\in BV([0,T],\mathbb{R})$. Then for every $\psi_0\in\mathcal{H}, t\in[0,T]$ the map $\Upsilon_t(\psi_0) : u\mapsto \Upsilon_t^u(\psi_0)\in\mathcal{H}$ admits a unique continuous extension on $\mathcal{R}((0,T])$ denoted $\Upsilon_t(\psi_0)$ which satisfies, for every u in $\mathcal{R}(I)$,*

$$\Upsilon_t^u(\psi_0) = e^{u((0,t])B}Y_t^u(\psi_0), \forall u\in\mathcal{R}((0,T]), \forall t\in[0,T].$$

From the above expression, we can see that the factor $e^{u((0,t])B}$ supports all the discontinuities of the solution. More precisely, the jumps of the solutions are the atoms of u.

Making a crucial use of Helly's selection theorem, we obtained among others the results of the previous section. Actually the case of bounded operator was treated separately and the existence theory in the Radon case was obtained directly from a Dyson type expansion allowing less assumptions on (A,B).

6.5.2 The new form of the weak coupling

The weak coupling was then reformulated as in the following

Definition 6.21 (Weakly coupled)**.** *Let k be a non negative real. A couple of* skew-adjoint *operators (A,B) is k-*weakly coupled *if*

1. *A is invertible with bounded inverse from $D(A)$ to $\mathcal{H}$*
2. *for any real t, $e^{tB}D(|A|^{k/2})\subset D(|A|^{k/2})$,*
3. *there exists $c\geq 0$ and $c'\geq 0$ such that $B-c$ and $-B-c'$ generate contraction semigroups on $D(|A|^{k/2})$ for the norm $\psi\mapsto \||A|^{k/2}u\|$.*

In [BCC14c], we provided different equivalent definitions and showed that the former definition of weak-coupling actually implied the new one.

The main interest of this definition is to show that the weak-coupling is in fact almost a restatement in $D(|A|^k)$ of the assumption we made in $\mathcal{H}$ to ensure the well posedness of (6.1). This lead us to the

Proposition 6.22. *Let k be a non negative real. Let (A,B) be k-weakly coupled and B be A-bounded.*

For any $u\in BV([0,T],\mathbb{R})\cap B_{L^\infty([0,T])}(0,1/\|B\|_A)$, there exists a family of contraction propagators in $\mathcal{H}$ that extends uniquely as contraction propagators to $D(|A|^{k/2})$: $\Upsilon^u : \Delta_{[0,T]}\to L(D(|A|^{k/2}))$ such that

1. *for any $t\in[0,T]$, for any $\psi_0\in D(|A|^{k/2})$*

$$\|\Upsilon_t(\psi_0)\|_{k/2} \leq e^{c_k(A,B)\int_0^t |u|}\|\psi_0\|_{k/2}$$

2. for any $t \in [0,T]$, for any $\psi_0 \in D(|A|^{1+k/2})$ for any $u \in BV([0,T],\mathbb{R})$ with $\|u\|_\infty < 1/\|B\|_A$), there exists m (depending only on A, B and $\|u\|_{L^\infty([0,T])}$)

$$\|\Upsilon_t(\psi_0)\|_{1+k/2} \leq m e^{m\|u\|_{BV([0,T],\mathbb{R})}} e^{c_k(A,B)\int_0^t |u|} \|\psi_0\|_{1+k/2}$$

Moreover, for every ψ_0 in $D(|A|^{k/2})$, the end-point mapping

$$\begin{aligned}\Upsilon(\psi_0) : BV([0,T],K) &\to D(|A|^{k/2})\\ u &\mapsto \Upsilon^u(0,T)(\psi_0)\end{aligned}$$

is continuous.

Then our main point was that any statement that we made in $\mathcal{H}$ in the bounded variation case still holds in $D(|A|^{k/2})$ when (A,B) is k-weakly coupled. The Radon measure case cannot be attained as the interacting framework is more demanding in terms of regularity. Instead, we obtained the results by interpolating $\mathcal{H}$ and $D(|A|^{k/2})$ which gave the space $D(|A|^s)$ for $s \in [0,k/2)$. In this case we can thus extend the result we obtain in $\mathcal{H}$ to $D(|A|^s)$ for $s \in [0,k/2)$.

6.5.3 Operators with a non pure point spectrum

When the operator A does not admit a basis of eigenvectors some parts of the theory in Section 6.3 do not extend easily. It does not necessarily mean that we cannot reach some of the conclusion we made.

For instance, we can make use of the

Theorem 6.23 (Weyl-Von Neumann)**.** *Let A be a skew-adjoint operator on $\mathcal{H}$. For any $\varepsilon > 0$, there exists $C_\varepsilon \in \mathcal{B}_2(\mathcal{H})$ skew-adjoint with $\|C_\varepsilon\|_2 \leq \varepsilon$ and such that $A + C_\varepsilon$ has pure point spectrum.*

With this tool we can for instance obtain good Galerkin approximations and then use finite dimensional theory and expect some interesting controllability results. We have thus the

Proposition 6.24. *Let A be skew-adjoint, B be bounded with $B(1-A)^{-1}$ compact and s be in $[0,1)$. Then for every $\varepsilon > 0$, $L \geq 0$, $T > 0$, $n \in \mathbb{N}$, and $(\psi_j)_{1\leq j\leq n}$ in $D(|A|^{k/2})^n$ there exists a Hilbert basis Φ of $\mathcal{H}$ and $N \in \mathbb{N}$ such that for any $u \in BV(0,T]$,*

$$|u|([0,T]) < L \Rightarrow \|\Upsilon^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N\psi_j\|_{s/2} < \varepsilon,$$

for every t in $[0,T]$ and $j = 1,\dots,n$.

References

[AG74] W. O. Amrein and V. Georgescu. “ On the characterization of bound states and scattering states in quantum mechanics ”. In: *Helv. Phys. Acta* 46 (1973/74), pp. 635–658.

[BCC12a] N. Boussaïd, M. Caponigro, and T. Chambrion. “ Approximate controllability of the Schrödinger equation with a polarizability term ” . In: *Decision and Control (CDC), 2012 IEEE 51st Annual Conference on.* IEEE. 2012, pp. 3024–3029. DOI: 10.1109/CDC.2012.6426619. URL: http://hal.archives-ouvertes.fr/hal-00784881/PDF/Quadratique13.pdf.

[BCC12b] N. Boussaïd, M. Caponigro, and T. Chambrion. " Implementation of logical gates on infinite dimensional quantum oscillators ". In: *American Control Conference (ACC), 2012*. IEEE. 2012, pp. 5825–5830. URL: http://hal.archives-ouvertes.fr/hal-00637115/PDF/QG%5C_ACC%5C_0.6.pdf.

[BCC12c] N. Boussaïd, M. Caponigro, and T. Chambrion. " Periodic control laws for bilinear quantum systems with discrete spectrum ". In: *American Control Conference (ACC), 2012*. IEEE. 2012, pp. 5819–5824. URL: http://hal.archives-ouvertes.fr/hal-00637116/PDF/FEPS%5C_ACC%5C_3.pdf.

[BCC12d] N. Boussaïd, M. Caponigro, and T. Chambrion. " Small time reachable set of bilinear quantum systems " . In: *Decision and Control (CDC), 2012 IEEE 51st Annual Conference on*. IEEE. 2012, pp. 1083–1087. DOI: 10.1109/CDC.2012.6426208. URL: http://hal.archives-ouvertes.fr/hal-00710040/PDF/Time06.pdf.

[BCC12e] N. Boussaïd, M. Caponigro, and T. Chambrion. " Which notion of energy for bilinear quantum systems? " In: *proceeding of the 4th IFAC Workshop on Lagrangian and Hamiltonian Methods for Non Linear Control, pp 226-230, 29-31 août 2012*. 2012, pp. 226–230. DOI: 10.3182/20120829-3-IT-4022.00034. URL: http://hal.archives-ouvertes.fr/hal-00784890/PDF/Energy4.pdf.

[BCC13a] N. Boussaïd, M. Caponigro, and T. Chambrion. " Energy Estimates for Low Regularity Bilinear Schrödinger Equations " . In: *Control of Systems Governed by Partial Differential Equations*. Vol. 1. 1. 2013, pp. 25–30. DOI: 10.3182/20130925-3-FR-4043.00046. URL: http://hal.archives-ouvertes.fr/hal-00784876/PDF/cpde09.pdf.

[BCC13b] N. Boussaïd, M. Caponigro, and T. Chambrion. " Total variation of the control and energy of bilinear quantum systems " . In: *Decision and Control (CDC), 2013 IEEE 52nd Annual Conference on*. Dec. 2013, pp. 3714–3719. DOI: 10.1109/CDC.2013.6760455. URL: http://hal.archives-ouvertes.fr/hal-00800548/PDF/BVefficiency09.pdf.

[BCC13c] N. Boussaïd, M. Caponigro, and T. Chambrion. " Weakly coupled systems in quantum control " . In: *IEEE Trans. Automat. Control* 58.9 (2013), pp. 2205–2216. DOI: 10.1109/TAC.2013.2255948.

[BCC14a] N. Boussaïd, M. Caponigro, and T. Chambrion. *Approximate controllability of the Schrödinger Equation with a polarizability term in higher Sobolev norms*. June 2014. URL: http://hal.archives-ouvertes.fr/hal-01006178.

[BCC14b] N. Boussaïd, M. Caponigro, and T. Chambrion. *Efficient finite dimensional approximations for the bilinear Schrodinger equation with bounded variation controls*. 2014. URL: http://hal.archives-ouvertes.fr/hal-01003056.

[BCC14c] N. Boussaïd, M. Caponigro, and T. Chambrion. *Regular propagators of bilinear quantum systems*. June 2014. URL: http://hal.archives-ouvertes.fr/hal-01016299.

[BCT14] K. Beauchard, J.-M. Coron, and H. Teismann. " Minimal time for the bilinear control of Schr\"odinger equations ". In: *ArXiv e-prints* (Jan. 2014). arXiv: 1401.6828 [math.AP].

[Bea05] K. Beauchard. " Local controllability of a 1-D Schrödinger equation ". In: *J. Math. Pures Appl.* 84.7 (2005), pp. 851–956.

[BL10] K. Beauchard and C. Laurent. " Local controllability of 1D linear and nonlinear Schrödinger equations with bilinear control ". In: *J. Math. Pures Appl.* 94.5 (2010), pp. 520–554.

[BMS82] J. M. Ball, J. E. Marsden, and M. Slemrod. " Controllability for distributed bilinear systems ". In: *SIAM J. Control Optim.* 20.4 (1982), pp. 575–597.

[Bos+12] U. Boscain, M. Caponigro, T. Chambrion, and M. Sigalotti. " A weak spectral condition for the controllability of the bilinear Schrödinger equation with application to the control of a rotating planar molecule ". In: *Comm. Math. Phys.* 311.2 (2012), pp. 423–455.

[Cha+09] T. Chambrion, P. Mason, M. Sigalotti, and U. Boscain. " Controllability of the discrete-spectrum Schrödinger equation driven by an external field ". In: *Ann. Inst. H. Poincaré Anal. Non Linéaire* 26.1 (2009), pp. 329–349.

[Cha12] T. Chambrion. " Periodic excitations of bilinear quantum systems " . In: *Automatica J. IFAC* 48.9 (2012), pp. 2040–2046. DOI: 10.1016/j.automatica.2012.03.031. URL: http://dx.doi.org/10.1016/j.automatica.2012.03.031.

[Ens78] V. Enss. " Asymptotic completeness for quantum mechanical potential scattering. I. Short range potentials ". In: *Comm. Math. Phys.* 61.3 (1978), pp. 285–291.

[Kat53] T. Kato. " Integration of the equation of evolution in a Banach space ". In: *J. Math. Soc. Japan* 5 (1953), pp. 208–234.

[Kat70] T. Kato. " Linear evolution equations of "hyperbolic" type ". In: *J. Fac. Sci. Univ. Tokyo Sect. I* 17 (1970), pp. 241–258.

[MR04] M. Mirrahimi and P. Rouchon. " Controllability of quantum harmonic oscillators " . In: *IEEE Trans. Automat. Control* 49.5 (2004), pp. 745–747. DOI: 10.1109/TAC.2004.825966. URL: http://dx.doi.org/10.1109/TAC.2004.825966.

[Nat55] I. P. Natanson. *Theory of functions of a real variable.* Translated by Leo F. Boron with the collaboration of Edwin Hewitt. 1955, p. 277.

[Ner09] V. Nersesyan. " Growth of Sobolev norms and controllability of the Schrödinger equation ". In: *Comm. Math. Phys.* 290.1 (2009), pp. 371–387.

[Rue69] D. Ruelle. " A remark on bound states in potential-scattering theory ". In: *Nuovo Cimento A (10)* 61 (1969), pp. 655–662.

[Tur00] G. Turinici. " On the controllability of bilinear quantum systems ". In: *Mathematical models and methods for ab initio Quantum Chemistry*. Ed. by M. Defranceschi and C. Le Bris. Vol. 74. Lecture Notes in Chemistry. 2000.

III.7

Stability of non-linear Dirac problems

In this section, we present the results of the analysis [BC12c; BC12b], in which we considered the stability problem related to non-linear Dirac models. This is the chapter which is the most related to my PhD work. I've chosen to present first the joint work with Andrew Comech on the spectral and linear stability and then the one with Scipio Cuccagna on the non-linear stability. This is opposite to the chronological order but in a sense the spectral analysis should precede the non-linear analysis.

This situation is explained as follows: the spectral analysis is a difficult analysis with very limited outcome. In many situations it has to be accompanied by numerical evidences. We choose with Scipio Cuccagna to proceed further paying the price of making assumptions on the linearised spectrum.

We mention that we provide a limited bibliography in the sequel. The actual bibliography in this field is limited. The non-linear Dirac equation due to its strong indefiniteness cannot be analysed from the stability point of view with the tools introduced for its non-relativistic counter part: the non-linear Schrödinger equation. For instance the orbital stability which was obtained either by concentration-compactness method [CL82] or by Lyapounov methods [GSS87] for the non-linear Schrödinger equations can no longer be obtained by these means for the non-linear Dirac equations.

7.1 The spectral stability of dispersive relativistic models

This section presents the analysis [BC12b] in collaboration with Andrew Comech.

We considered the non-linear Dirac equation

$$\mathrm{i}\partial_t u = D_m u - g(u\overline{u})\beta u, \qquad \psi(x,t) \in \mathbb{C}^N, \quad x \in \mathbb{R}^n, \tag{NLDE}$$

where $g \in C(\mathbb{R})$ with $g(0) = 0$ and $\overline{u} = \beta u^*$ ($\cdot^*$ denoted the complex conjugation).

The non-linearity is such that the equation is $\mathbf{U}(1)$-invariant. If $\phi_\omega(x)e^{-\mathrm{i}\omega t}$ is a solitary wave solution to (NLDE), then the profile ϕ_ω satisfies the stationary equation

$$\omega\phi = D_m\phi - g(\phi^*\beta\phi)\beta\phi. \tag{7.1}$$

In order to avoid any discussion on the existence of solitary waves and to restrict our assumptions to what is needed for the analysis of the spectral stability, we made the

Assumption 7.1.1. *There exists a nonempty open interval $\mathcal{O} \subseteq (-m, m)$ such that equation (7.1) admits a C^1 family of solutions $\omega \mapsto \phi_\omega$, $\mathcal{O} \to H^s(\mathbb{R}^n)$, for some $s > n/2$.*

One of our main tool is a version of the Carleman inequality for the Dirac operator due to Berthier and Georgescu [BG87], which we extended to any dimension. In order to formulate it, for $\lambda \in \mathbb{R} \setminus [-m, m]$ and for constants $M \geq 1$, $\mathcal{N} \geq 1$, $\rho \geq 1$, and $\nu > 0$, we introduce the set of functions

$$\mathscr{C}_\lambda(M, \mathcal{N}, \rho, \nu) = \Big\{ \varphi \in C^2(\mathbb{R}_+) \ ; \ \ \varphi' > 0,\, 0 < \varphi' \leq \mathcal{N} r,\, r|\varphi''| \leq M\varphi', \\ \lambda^2 - m^2 + \varphi'^2 + 2r\varphi'\varphi'' \geq \nu \quad \text{for} \ \ r \geq \rho \Big\}.$$

Theorem 7.1 (Carleman–Berthier–Georgescu inequality in $\mathbb{R}^n$)**.** *Let $n \in \mathbb{N}$, $m > 0$, and $\varphi \in C^2(\mathbb{R}_+)$. Let $\lambda \in \mathbb{R} \backslash [-m, m]$. Assume that*

$$\varphi \in \mathscr{C}_\lambda(M, \mathcal{N}, \rho, \nu)$$

for some M, $\mathcal{N}$, $\rho \geq 1$, and $\nu > 0$. Denote

$$\mu(r) = 8\sqrt{n + \lambda^2} \left(\sqrt{1 + r\varphi'(r)} + \frac{r}{\sqrt{1 + r\varphi'(r)}} \right).$$

There is $R_0(M, m, n, \lambda) < \infty$ such that for any $u \in H^1(\mathbb{R}^n, \mathbb{C}^N)$ with $\operatorname{supp} u \subset \Omega_R$ and $R \geq \max(\rho, R_0(M, m, n, \lambda))$, which satisfies

$$\mu e^{\varphi}(D_m - \lambda)u \in L^2(\mathbb{R}^n, \mathbb{C}^N),$$

one has $(\lambda^2 - m^2 + \varphi'^2 + 2r\varphi'\varphi'')^{1/2} e^{\varphi} u \in L^2(\mathbb{R}^n, \mathbb{C}^N)$, and moreover

$$\left\| \left(\lambda^2 - m^2 + \varphi'^2 + 2r\varphi'\varphi''\right)^{1/2} e^{\varphi} u \right\|^2 \leq 2 \left\| \mu e^{\varphi}(D_m - \lambda)u \right\|^2.$$

Note that φ is considered as a function of $|x|$.

The above theorem has many consequences for the analysis of eigenvectors and sequence of eigenvectors. As an illustration we have the

Theorem 7.2 (Properties of solitary wave solutions)**.** *Let $n \in \mathbb{N}$.*

1. *Let Assumption 7.1.1 be satisfied. Let ϕ_ω, $\omega \in \mathcal{O}$, be a solution to (7.1). Then for any $\mu < \sqrt{m^2 - \omega^2}$ one has $e^{\mu\langle Q \rangle}\phi_\omega \in L^2(\mathbb{R}^n, \mathbb{C}^N)$.*

2. *Let $g \in C(\mathbb{R})$. For $\omega \in \mathbb{R} \backslash [-m, m]$, there are no solitary wave solutions $\phi_\omega(x)e^{-\mathrm{i}\omega t}$ to (NLDE) such that $\phi_\omega \in L^2(\mathbb{R}^n, \mathbb{C}^N) \cap H^1_{\mathrm{loc}}(\mathbb{R}^n, \mathbb{C}^N) \cap L^\infty(\mathbb{R}^n, \mathbb{C}^N)$.*

We now explain the main steps of the proof of a simpler result. This is the core of some proofs we made.

Statement :

If $g(x) = o(|x|^2)$ then for $\omega > m$ then there is no solitary waves $\phi_\omega(x)e^{-i\omega t}$, such that $|x|^{1/4}\phi_\omega(x) \in L^\infty(\mathbb{R}^n, \mathbb{C}^N)$.

Sketched proof :

1. Using our assumption on g and ϕ_ω with Theorem 7.1, there exists $R_0 \geq 0$, $\tau_0 > 0$ and $C(R_0) > 0$ such that for any $R \geq R_0$, for any $u \in H_0^1(B(0,R)^c, \mathbb{C}^N)$, and for any $\tau \geq \tau_0$

$$\|e^{\tau r} u\|_{L^2(B(0,R)^c,\mathbb{C}^N)} \leq \frac{C(R_0)}{\tau} \left\| r^{1/2} e^{\tau r}(D_m - g(\phi_\omega^* \beta \phi_\omega)\beta - \omega)u \right\|_{L^2(B(0,R)^c,\mathbb{C}^N)}.$$

2. Consider $v_j = \eta_j \phi$ with $\eta_j := \eta(\cdot/j)$, where $\eta \in C^\infty(\mathbb{R})$ satisfies $0 \leq \eta \leq 1$,

$$\eta(x) = 1, \text{ for } x \in B(0,2)^c \text{ and } 0 \text{ for } x \in B(0,1).$$

For $\tau > 1$ and for $j > R_0$ sufficiently large,

$$\begin{aligned}\|e^{\tau r} v_j\|_{L^2(B(0,R)^c,\mathbb{C}^N)} &\leq \frac{2C(R_0)}{\tau} \left\| r^{1/2} e^{\tau r}(D_m - g(\phi_\omega^* \beta \phi_\omega)\beta - \omega)v_j \right\|_{L^2(B(0,R)^c,\mathbb{C}^N)} \\ &\leq \frac{2C(R_0)}{\tau} \left\| r^{1/2} e^{\tau r} \alpha \cdot (\nabla \eta_j)\phi_\omega \right\|_{L^2(B(0,R)^c,\mathbb{C}^N)},\end{aligned}$$

which implies that

$$e^{\tau 3j} \|\phi_\omega\|_{L^2(B(0,3j)^c,\mathbb{C}^N)} \leq \text{const} \frac{2C(R_0)}{\tau} e^{\tau 2j} \|\phi_\omega\|_{L^2(B(0,j)^c \cap B(0,2j)^c,\mathbb{C}^N)}.$$

Considering $\tau \to \infty$ leads to ϕ_ω is identically zero outside of the ball B_{3j}.

3. We use a unique continuation principle for the Dirac operator to conclude. □

7.1.1 The linearised operator

The linearised operator is obtain trough a linear approximation of the flow in a vicinity of an equilibrium. A stationary solution can be turned to an equilibrium by a simple time dependent change of gauge. For instance, we considered solutions to (NLDE) in the form of the Ansatz $u(x,t) = (\phi_\omega(x) + \rho(x,t))e^{-\mathrm{i}\omega t}$, so that $\rho(x,t) \in \mathbb{C}^N$ is a small perturbation of the solitary wave. *If g is Fréchet differentiable at values of $\phi_\omega^* \beta \phi_\omega$, but not necessarily at zero,* (e.g. $g(s) = |s|^k$ with $k > 0$), the linearisation at the solitary wave $\phi_\omega(x)e^{-\mathrm{i}\omega t}$ (the linearised equation on ρ) is given by

$$\mathrm{i}\partial_t \rho = \mathcal{L}(\omega)\rho, \tag{7.2}$$

where

$$\mathcal{L}(\omega) = D_m - \omega - g(\phi_\omega^* \beta \phi_\omega)\beta - 2g'(\phi_\omega^* \beta \phi_\omega)\beta \phi_\omega \Re(\phi_\omega^* \beta\ \cdot).$$

The operator $\mathcal{L}(\omega)$ is not $\mathbb{C}$-linear because of the term with $\Re(\phi_\omega^* \beta\ \cdot)$. To work with $\mathbb{C}$-linear operators, we introduced

$$\boldsymbol{\alpha}^\jmath = \begin{bmatrix} \Re\alpha^\jmath & -\Im\alpha^\jmath \\ \Im\alpha^\jmath & \Re\alpha^\jmath \end{bmatrix}, \quad 1 \leq \jmath \leq n; \qquad \boldsymbol{\beta} = \begin{bmatrix} \Re\beta & -\Im\beta \\ \Im\beta & \Re\beta \end{bmatrix}, \qquad \mathbf{J} = \begin{bmatrix} 0 & I_N \\ -I_N & 0 \end{bmatrix},$$

where the real part of a matrix is the matrix made of the real part of its entries (and similarly for the imaginary part of a matrix). For

$$\boldsymbol{\phi}_\omega(x) = \begin{bmatrix} \Re\phi_\omega(x) \\ \Im\phi_\omega(x) \end{bmatrix} \in \mathbb{R}^{2N}$$

and $\mathbf{D}_m = \mathbf{J}\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + m\boldsymbol{\beta}$ the operator corresponding to D_m acting on $\mathbb{R}^{2N}$-valued functions, we introduced the operator

$$\mathbf{L}(\omega) = \mathbf{D}_m - \omega - g(\boldsymbol{\phi}_\omega^*\boldsymbol{\beta}\boldsymbol{\phi}_\omega)\boldsymbol{\beta} - 2(\boldsymbol{\phi}_\omega^*\boldsymbol{\beta}\ \cdot)g'(\boldsymbol{\phi}_\omega^*\boldsymbol{\beta}\boldsymbol{\phi}_\omega)\boldsymbol{\beta}\boldsymbol{\phi}_\omega.$$

by $\mathbb{C}$-linearity, it extends onto

$$\mathscr{X} = H^1(\mathbb{R}^n, \mathbb{C}^{2N}) = H^1(\mathbb{R}^n, \mathbb{C}\otimes_{\mathbb{R}}\mathbb{R}^{2N}),$$

and in order for it to be be self-adjoint on the domain $H^1(\mathbb{R}^n, \mathbb{C}^{2N})$, we assume that

$$\boxed{f'(x) = o(\frac{1}{|x|}) \text{ as } x \to 0.}$$

The linearisation at the solitary wave (7.2) takes the form

$$\partial_t\boldsymbol{\rho} = \mathbf{J}\mathbf{L}(\omega)\boldsymbol{\rho}, \qquad \boldsymbol{\rho}(x,t) = \begin{bmatrix}\Re\rho(x,t)\\ \Im\rho(x,t)\end{bmatrix} \in \mathbb{R}^{2N} \tag{7.3}$$

where $\mathbf{J}$ acts as

$$\begin{pmatrix} 0 & I_N \\ -I_N & 0\end{pmatrix}.$$

Recall the following

Definition 7.3. *We will say that a particular solitary wave is* linearly stable *if the spectrum of the equation linearised at this wave does not contain points with positive real part and if there are no 4×4 Jordan blocks at $\lambda = 0$ and no 2×2 Jordan blocks at $\lambda \in \mathrm{i}\mathbb{R}\setminus 0$.*

This definition is reminiscent of Definition 7.7 below. There is only one extra requirements in the later that we comment in the sequel.

The essential spectrum of $\mathbf{J}\mathbf{L}(\omega)$ is purely imaginary, with the edges at the thresholds $\pm(m-|\omega|)\mathrm{i}$ (this is a consequence of Weyl's theorem). There are also embedded thresholds $\pm(m+|\omega|)\mathrm{i}$. Hence from the point of view of linear stability, we were only interested in the point spectrum of this operator.

Let us be more precise on this last comment. At this point of our investigations, we haven't consider the question of the dispersive properties of the linearised operator on the essential spectrum. From the point of view of the stability, as long as we do not seek optimal estimates, we can consider the Kato smoothness and Strichartz estimates of Part II. It won't be sufficient but Kato smoothness will follow from a limiting absorption principle that we are currently investigating. Then as $f(0) = 0$ and if $f'(x) = o(|x|^{-1-\epsilon})$, $\epsilon > 0$, due to the exponential decay of ϕ_ω, see Theorem 7.2, a perturbation approach will lead to Strichartz estimates.

In order to attain attain an optimal setting, it will be interesting to consider estimates for non-autonomous linearised operators.

7.1.2 Linearised spectrum of the non-linear Schrödinger operator

In order to explain our results it maybe relevant to recall an important fact on the non-linear Schrödinger equation.

For the ground state solution $\phi_\omega(x)e^{-\mathrm{i}\omega t}$ to the non-linear Schrödinger equation

$$\mathrm{i}\partial_t\psi = -\Delta\psi - |\psi|^{2k}\psi, \qquad \psi(x,t)\in\mathbb{C}, \quad x\in\mathbb{R}^n, \tag{NLS}$$

where $k > 0$, the linearisation is given by

$$\partial_t \rho = \mathbf{j}\ell(\omega)\rho,$$

where

$$(\mathbf{j} = 1/i,) \qquad \ell(\omega) = \ell_-(\omega) - 2k\Re(\phi_\omega{}^* \cdot)|\phi_\omega|^{2(k-1)}\phi_\omega, \quad \ell_-(\omega) = -\Delta - \omega - |\phi_\omega|^{2k}.$$

This operator acts on $\mathbb{R}^2$ valued function instead of $\mathbb{C}$. The real space $\mathbb{R}^2$ is then embedded in $\mathbb{C}^2$. The extension of $\mathbf{j}\ell(\omega)$ reads as

$$\mathbf{j}\mathbf{l}(\omega) := \begin{pmatrix} 0 & \ell_-(\omega) \\ -\ell(\omega) & 0 \end{pmatrix}.$$

We have that $\ell_-(\omega)\phi_\omega = 0$ so that from Perron-Frobenius and Sturm oscillation theorems $\ell_-(\omega) > cI_{\phi_\omega^\perp}$ for some $c > 0$. Hence $\mathbf{j}\mathbf{l}(\omega)\rho = \lambda\rho$ implies

$$\sqrt{\ell_-(\omega)}\ell(\omega)\sqrt{\ell_-(\omega)}R = -\lambda^2 R$$

for $R = \sqrt{\ell_-(\omega)}\rho_2$ where ρ_2 is the second component of ρ, which is necessarily nonzero. If $\lambda \neq 0$ then $\lambda^2 \in \mathbb{R}$ and thus

$$\sigma(\mathbf{j}\mathbf{l}) \subset \mathbb{R} \cup \mathrm{i}\mathbb{R}. \tag{7.4}$$

7.1.3 The case of the linearised Dirac equations

The property 7.4 seems no longer true for Dirac type models so we tried to recover part of this property or at least to analyse the behaviour of sequences associated to the complementary set of $\mathbb{R} \cup \mathrm{i}\mathbb{R}$.

The $\pm 2\omega\mathrm{i}$ eigenvalues. At this point, we can mention another difficulty coming from the matrix aspect of the Dirac operator. The spectrum of a linearised operator, always contains the points $\pm 2\omega\mathrm{i}$ as stated by

Lemma 7.4. *Let α^0 be an hermitian matrix anti-commuting with $\alpha^\jmath$, $1 \leq \jmath \leq n$, and with β. Then $\alpha^0\phi_\omega$ is an eigenfunction of $\mathcal{L}_-$ and of $\mathcal{L}$, corresponding to the eigenvalue $\lambda = -2\omega$ and it follows that*

$$\pm 2\omega\mathrm{i} \in \sigma_p(\mathbf{j}\mathcal{L}(\omega)).$$

If n is odd α^0 can be the product of $\alpha^\jmath$, $1 \leq \jmath \leq n$, and β. In the other case, we have to consider spatial symmetries and use symmetries of ϕ_ω and g.

These eigenvalues are always present in the spectrum of the linearised operator and represents a serious obstacle to the stability analysis. To understand this we defined in a work in progress with Andrew Comech the following

$$\chi_\omega := \alpha^0\phi_\omega;$$

then, applying α^0 to (7.1), we see that χ_ω satisfies

$$-\omega\chi_\omega = D_m\chi_\omega - f(\phi_\omega^*\beta\phi_\omega)\beta\chi_\omega = D_m\chi_\omega - f(-\chi_\omega^*\beta\chi_\omega)\beta\chi_\omega. \tag{7.5}$$

If $f(s)$ is even, then $\chi e^{\mathrm{i}\omega t}$ is a solitary wave solution to (NLDE).

Let us assume that

$$\phi_\omega^*\beta\chi_\omega = \phi_\omega^*\beta\alpha^0\phi_\omega = 0.$$

This is for instance true for the solutions of the Soler model considered by [CV86]

Then for a, $b \in \mathbb{C}$ satisfy $|a|^2 - |b|^2 = 1$, define

$$\psi(x,t) = a\phi_\omega(x)e^{-\mathrm{i}\omega t} + b\chi_\omega(x)e^{\mathrm{i}\omega t}.$$

Taking up the linear combination of (7.1) and (7.5), we see that

$$\mathrm{i}\partial_t\psi = a\omega\phi_\omega e^{-\mathrm{i}\omega t} - b\omega\chi_\omega e^{\mathrm{i}\omega t} = D_m\psi - f(\psi^*\beta\psi)\beta\psi.$$

We took into account that

$$\begin{aligned}\psi^*\beta\psi &= (a\phi_\omega e^{-\mathrm{i}\omega t} + b\chi_\omega e^{\mathrm{i}\omega t})^*\beta(a\phi_\omega e^{-\mathrm{i}\omega t} + b\chi_\omega e^{\mathrm{i}\omega t}) \\ &= (|a|^2 - |b|^2)\phi_\omega^*\beta\phi_\omega.\end{aligned}$$

We obtained a manifold of bi-frequency solitary waves of the form

$$\mathscr{M} = \left\{e^{\mathrm{i}\vartheta}(a\phi_\omega + b\chi_\omega)\ ; \quad \vartheta \in \mathbb{T}, \quad b \in \mathbb{C}^1, \quad a = \sqrt{1+|b|^2}, \quad \omega \in \mathcal{O}\right\}.$$

This is a manifold of solutions larger than the manifold of stationary solutions. An orbit of this manifold never intersects the orbit of a stationary solution unless it is the orbit of a stationary solution. This manifold has to replace the curve $\omega \mapsto \phi_\omega$ in the stability analysis. Below we consider a larger class of perturbations of Dirac operators containing the class of linearised operator. The following considerations are still valid for linearisation around solutions in $\mathscr{M}$. The time dependent problem and especially the modulations of the term b still have to be investigated.

7.1.4 Embedded point spectrum

We formulated our results on the point spectrum for the operator JL, where

$$L = D_m - \omega + V, \qquad \omega \in (-m, m),$$

$V : \mathbb{R}^n \to \mathrm{End}\,(\mathbb{C}^N)$ is measurable, and such that there is $\tau_0 > 0$ and $C < \infty$ with

$$\sup_{x\in\mathbb{R}^n} \left\| e^{\tau_0|x|}V(x)\right\|_{\mathbb{C}^N\to\mathbb{C}^N} < C$$

and J is a skew symmetric $2N \times 2N$ matrix such that $J^2 = -I_{2N}$. Notice that we did not assume that V is hermitian valued.

With Theorem 7.1 and a limiting absorption principle, we proved the

Theorem 7.5 (Properties of embedded eigenstates)**.** *Let $n \geq 1$. Let $J \in \mathrm{End}\,(\mathbb{C}^N)$ be skew-adjoint and invertible, $J^2 = -1$, $[J, D_m] = 0$. Assume that there is $\tau_0 > 0$ such that*

$$\sup_{x\in\mathbb{R}^n} \left\| e^{\tau_0|x|}V(x)\right\|_{\mathrm{End}\,(\mathbb{C}^N)} < \infty.$$

1. *Let $\omega \in \mathcal{O}$, $\lambda \in \sigma_{\mathrm{p}}(JL(\omega)) \cap \mathrm{i}\mathbb{R}$, $|\lambda| < m + |\omega|$, $|\lambda| \neq m - |\omega|$. Then the corresponding eigenfunctions are exponentially decaying.*

2. *There are no embedded eigenvalues beyond the embedded thresholds $\pm\mathrm{i}(m + |\omega|)$:*

$$\sigma_{\mathrm{p}}(JL(\omega)) \cap \mathrm{i}(\mathbb{R}\backslash[-m - |\omega|, m + |\omega|]) = \emptyset.$$

Then we analysed the birth of eigenvalues with nonzero real part. As in Theorem 7.5, we formulated the results for general Dirac-type operators, having in mind the linearisation (7.3) of the non-linear Dirac equation or linearisation of (NLDE) around point in $\mathscr{M}$. We obtained the

Theorem 7.6 (Bifurcation of point eigenvalues). *Let $n \geq 1$. Let $J \in \operatorname{End}(\mathbb{C}^N)$ be skew-adjoint and invertible, $J^2 = -1$, $[J, D_m] = 0$. Let $(\omega_j)_{j\in\mathbb{N}}$, $\omega_j \in \mathcal{O}$, be a Cauchy sequence, $\omega_j \to \omega_b \in \mathcal{O}$, and assume that there is $\varepsilon > 0$ such that*

$$\left\|\langle Q\rangle^{1+\varepsilon} V(\omega_b)\right\|_{L^\infty(\mathbb{R}^n, \operatorname{End}(\mathbb{C}^{2N}))} < \infty, \qquad \lim_{j\to\infty} \left\|\langle Q\rangle^{1+\varepsilon} \left(V(\omega_j) - V(\omega_b)\right)\right\|_{L^\infty(\mathbb{R}^n, \operatorname{End}(\mathbb{C}^{2N}))} = 0.$$

Let $\lambda_j \in \sigma_{\mathrm{p}}(JL(\omega_j))$ be a Cauchy sequence, with $\lambda_j \underset{j\to\infty}{\longrightarrow} \lambda_b \in \mathrm{i}\mathbb{R}$. Then:

1. $|\lambda_b| \leq m + |\omega_b|$.
2. *If $|\lambda_b| < m + |\omega_b|$ and moreover V is hermitian, then*

$$\lambda_b \in \sigma_{\mathrm{p}}(JL(\omega_b)),$$

and there is a subsequence of eigenfunctions $(\zeta_j)_{j\in\mathbb{N}}$ corresponding to eigenvalues $\lambda_j \in \sigma_{\mathrm{p}}(JL(\omega_j))$ which converges in L^2 to the eigenfunction ζ_b corresponding to $\lambda_b \in \sigma_{\mathrm{p}}(JL(\omega_b))$.

Moreover, if there is a subsequence of $(\lambda_j)_{j\in\mathbb{N}}$ such that $\lambda_j \to \lambda_b$ and $\Re\lambda_j \neq 0$, then

$$\langle \zeta_b, L(\omega_b)\zeta_b\rangle = 0, \qquad \langle \zeta_b, J\zeta_b\rangle = 0.$$

The quantity $\langle \zeta_b, L(\omega_b)\zeta_b\rangle = 0$ is called Krein signature. Hence points of instability bifurcation are zero Krein signature eigenvalues. The reason for that is quite simple, the eigenvalues with nonzero real parts have zero Krein signature. So the same is true at the limits. As we also have $\langle \zeta_b, J\zeta_b\rangle = 0$, and hence if, as in Definition 7.7, we assume $\langle \zeta_b, J\zeta_b\rangle \neq 0$ this is an obstruction to the appearance of unstable directions from the embedded eigenvalues.

To sum-up, there is no embedded eigenvalues beyond the embedded thresholds and if eigenvalues bifurcate into the complex plane it is necessarily from an eigenvalue with zero Krein signature between the embedded thresholds.

Even if they are in a way simple to state the proofs of these results rely on an refined analysis of the ellipticity of the operators.

7.2 The asymptotic stability through resonances in the non-linear Dirac equation

We now present our analysis [BC12c] lead in collaboration with Scipio Cuccagna. We considered (NLDE) with $n = 3$ and $N = 4$ with the standard Dirac representation that is

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_{\mathbb{C}^2} & 0 \\ 0 & -I_{\mathbb{C}^2} \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Equation (NLDE) reads in this case

$$\begin{cases} \mathrm{i}u_t - D_m u + g(u\overline{u})\beta u = 0 \\ u(0,x) = u_0(x) \end{cases} (t,x) \in \mathbb{R}\times\mathbb{R}^3.$$

7.2.1 The assumptions on the symmetries and spectral stability

Once again, we decided to make *ad hoc* assumptions in order to consider the non-linear aspects. As mentioned the spectral aspects are still under investigation and our knowledge on that respect was even more limited at the time we worked on the analysis [BC12c] that we present now. At that time the numerical experiments made by [BC12a] were in agreement with our assumptions. We still think that these assumptions are valid

Let us start by presenting all the assumptions we made. It may look threatening but we gathered all the assumptions of a long analysis and a large part is either assumptions on the nonlinearity or symmetries imposed to the solitary waves or the initial conditions. Some of these assumptions, especially those on the symmetries, are are verified in some cases.

Below $C : \mathbb{C}^4 \to \mathbb{C}^4$ denotes the charge conjugation operator $u^c := Cu := \mathrm{i}\beta\alpha_2 u^*$. We have $\alpha_j C = C\alpha_j$ and $\beta C = -C\beta$ for all $j \in \{1, 2, 3\}$, see [Tha92, Sect. 1.4.6]. Since it is anti-linear, for any $u \in \mathbb{C}^4$, $C(u^*) = (Cu)^*$. We denoted by $\mathbf{L}(\omega, 0)$ the block diagonal operator

$$\begin{pmatrix} D_m - \omega & 0 \\ 0 & D_m + \omega \end{pmatrix}.$$

Let us recall the full set of assumptions we made.

(1) $g(0) = 0$, $g \in C^\infty(\mathbb{R}, \mathbb{R})$.

(2) There exists an open interval $\mathcal{O} \subseteq (m/3, m)$ such that $D_m u - \omega u - g(u\overline{u})\beta u = 0$ admits a C^∞ family of solutions $\omega \in \mathcal{O} \to \phi_\omega \in H^{k,\tau}(\mathbb{R}^3)$ for any (k, τ). In spherical coordinates $x_1 = \rho\cos(\vartheta)\sin(\varphi)$, $x_2 = \rho\sin(\vartheta)\sin(\varphi)$, $x_3 = \rho\cos(\varphi)$, these standing waves are of the form

$$\phi_\omega(x) = \begin{bmatrix} a(\rho) \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ \mathrm{i}b(\rho) \begin{bmatrix} \cos\varphi \\ e^{\mathrm{i}\vartheta}\sin\varphi \end{bmatrix} \end{bmatrix}$$

with $a(\rho)$ and $b(\rho)$ real valued and satisfying the following properties:

$$a, b \in C^\infty([0, \infty), \mathbb{R}), \quad \forall \rho \geq 0, \quad a^2(\rho) - b^2(\rho) \geq 0,$$
$$a^{(j)} \text{ and } b^{(j)} \text{ decay exponentially at infinity for all } j.$$

Notice that $\phi_\omega(-x) = \beta\phi_\omega(x)$ and $\phi_\omega(-x_1, -x_2, x_3) = S_3\phi_\omega(x_1, x_2, x_3)$ with $S_3 := \begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}$.

(3) Let $q(\omega) = \|\phi_\omega\|^2_{L^2}$. We assume $q'(\omega) \neq 0$ for all $\omega \in \mathcal{O}$.

(4) For any $x \in \mathbb{R}^3$ we consider in (NLDE) initial data s.t. $u_0(-x) = \beta u_0(x)$ and $u_0(-x_1, -x_2, x_3) = S_3 u_0(x_1, x_2, x_3)$.

(5) Let $\mathbf{L}(\omega)$ be the linearised operator around $e^{\mathrm{i}t\omega}\phi_\omega$. We assume that $\mathbf{L}(\omega)$ satisfies the

Definition 7.7 (Linear Stability)**.** *A standing wave $e^{\mathrm{i}t\omega}\phi_\omega$ is linearly stable when the following hold:*

(1) $\sigma(\mathrm{i}\mathbf{L}(\omega)) \subset \mathbb{R}$;

(2) $N_G(\mathrm{i}\mathbf{L}(\omega)) = \{\Sigma_3\Phi_\omega, \partial_\omega\Phi_\omega\}$;

(3) for any eigenvalue $z \neq 0$ *of* $\mathrm{i}\mathbf{L}(\omega)$ *we have* $N_G(\mathrm{i}\mathbf{L}(\omega) - z) = \mathrm{Ker}(\mathrm{i}\mathbf{L}(\omega) - z)$;

(4) for any positive eigenvalue $\lambda > 0$ *and for any* $\xi \in \mathrm{Ker}(\mathrm{i}\mathbf{L}(\omega) - \lambda)$, *we have* $\langle \xi, \Sigma_3 \xi^* \rangle > 0$.

If the positive discrete spectrum of $\mathrm{i}\mathbf{L}(\omega)$ is $0 < \lambda < \lambda_2 < \ldots < \lambda_n < \ldots$ then we fix an orthonormal basis $(\xi_{M_{n-1}+1}, \ldots, \xi_{M_{n-1}+m_n})$ of $\mathrm{Ker}(\mathrm{i}\mathbf{L}(\omega) - \lambda_n)$ where $m_0 = 0$, m_n is the multiplicity of λ_n and $M_n = \sum_{k=1}^{n} m_k$.

(6) Consider

$$\mathbf{X} := \big\{(\Upsilon_1, \Upsilon_2) \in L^2(\mathbb{R}^3, (\mathbb{C}^4)^2) : (\Upsilon_1(-x), \Upsilon_2(-x_1, -x_2, x_3) \equiv (\beta\Upsilon_1(x), -\beta\Upsilon_1(x), (\Upsilon_1(-x_1, -x_2, x_3), \Upsilon_2(-x_1, -x_2, x_3) \equiv (S_3\Upsilon_1(x), -S_3\Upsilon_1(x))\big\}.$$

The space $\mathbf{X}$ is invariant for the action of $\mathrm{i}\mathbf{L}(\omega)$. Consider the restriction of $\mathrm{i}\mathbf{L}(\omega)$ in $\mathbf{X}$. Then $\mathrm{i}\mathbf{L}(\omega)$ has $2n$ nonzero eigenvalues, counted with multiplicity, all contained in $(\omega - m, m - \omega)$. The positive eigenvalues can be listed as $0 < \lambda_1(\omega) \leq \ldots \leq \lambda_n(\omega) < m - \omega$, where we repeat each eigenvalue according to the multiplicity. For each $\lambda_j(\omega)$, also $-\lambda_j(\omega)$ is an eigenvalue. There are no other eigenvalues except for 0.

(7) The points and $\pm(m - \omega)$ and $\pm(m + \omega)$ are not resonances for $\mathrm{i}\mathbf{L}(\omega)$, see (7.6)–(7.7) below.

(8) Suppose that $\lambda \in \mathbb{R}$ with $|\lambda| > m - \omega$ is a resonance for $\mathrm{i}\mathbf{L}(\omega)$, that is one of the following two equations admits a nontrivial solution:

$$(1 + R^{+}_{\mathrm{i}\mathbf{L}(\omega,0)}(\lambda)V_\omega)u = 0, \quad u \in L^{2,-\tau}(\mathbb{R}^3, \mathbb{C}^8) \text{ for some } \tau > 1/2\ ; \tag{7.6}$$
$$(1 + R^{-}_{\mathrm{i}\mathbf{L}(\omega,0)}(\lambda)V_\omega)u = 0, \quad u \in L^{2,-\tau}(\mathbb{R}^3, \mathbb{C}^8) \text{ for some } \tau > 1/2\ . \tag{7.7}$$

Then if u satisfies either (7.6) or (7.7) we have $u \in L^2(\mathbb{R}^3, \mathbb{C}^8)$ and λ is an eigenvalue of $\mathrm{i}\mathbf{L}(\omega)$.

(9) There are natural numbers N_j defined by the property $0 < N_j\lambda_j(\omega) < m - \omega < (N_j + 1)\lambda_j(\omega)$.

(10) There is no multi index $\mu \in \mathbb{Z}^k$ with $|\mu| := |\mu_1| + \ldots + |\mu_k| \leq 2N_1 + 3$ such that $\mu \cdot \lambda = m \pm \omega$.

(11) If $\lambda_{j_1} < \ldots < \lambda_{j_k}$ are k distinct λ's, and $\mu \in \mathbb{Z}^k$ satisfies $|\mu| \leq 2N_1 + 3$, then we have

$$\mu_1\lambda_{j_1} + \cdots + \mu_k\lambda_{j_k} = 0 \iff \mu = 0\ .$$

(12) The non-linear Fermi golden rule holds at ω_0, that is for some fixed constant $C > 0$, for any vector $\zeta \in \mathbb{C}^n$ we have:

$$\sum_{\substack{\lambda^0\cdot\alpha=\lambda^0\cdot\nu>m-\omega_0 \\ \lambda\cdot\alpha-\lambda_k<m-\omega_0\,\forall k \text{ s.t. } \alpha_k\neq 0 \\ \lambda\cdot\nu-\lambda_k<m-\omega_0\,\forall k \text{ s.t. } \nu_k\neq 0}} \lambda^0 \cdot \nu \Im\left(\zeta^\alpha \overline{\zeta}^\nu \langle R^{+}_{\alpha 0} H^0_{\alpha 0}, \mathrm{i}\beta\alpha_2\Sigma_1\Sigma_3 H^0_{0\nu}\rangle\right) \geq C \sum_{\substack{\lambda^0\cdot\alpha>m-\omega_0 \\ \lambda^0\cdot\alpha-\lambda^0_k<m-\omega_0\,\forall k \text{ s.t. } \alpha_k\neq 0}} |\zeta^\alpha|^2.$$

where $R^{+}_{\mu 0} = (\mathrm{i}\mathbf{L}(\omega) - \lambda^0 \cdot \mu - \mathrm{i}0)^{-1}$ and

$$H^0_{\alpha 0} = \partial^\alpha \mathcal{G}(\phi_{\omega_0})\xi_\alpha$$

where for $\alpha \in \mathbb{N}^M$ ($M \in \mathbb{N} \cup \{\infty\}$ is the number of positive eigenvalues of $i\mathbf{L}(\omega)$) with $|\alpha| < \infty$, ξ_α is the $|\alpha|$-uple $(u_1, \ldots, u_{|\alpha|})$ formed such that

$$u_j = \xi_{\alpha_i} \text{ if } \sum_{k=1}^{i-1} \alpha_k \leq j < \sum_{k=1}^{i} \alpha_k.$$

and

$$H^0_{0\nu} = \partial^\alpha \nabla \mathcal{G}(\phi_\omega)(C\xi)_\nu$$

where $(C\xi)_\nu$ is built similarly yo ξ_ν with the $(C\xi_j)_{1\leq j\leq M}$ and

$$\mathcal{G}(U) = G(U^*\beta U)$$

where G is the an antederivative of g and

$$\Sigma_1 = \begin{pmatrix} 0 & I_{\mathbb{C}^4} \\ I_{\mathbb{C}^4} & 0 \end{pmatrix}, \Sigma_3 = \begin{pmatrix} I_{\mathbb{C}^4} & 0 \\ 0 & -I_{\mathbb{C}^4} \end{pmatrix}.$$

Assumption **(1)** is stronger than the one me made in the previous section. Assumption **(2)** is close to Assumption 7.1.1 especially when it is considered in conjunction with Theorem 7.2. Except for the smoothness with respect to the parameter ω, for some non-linearities **(2)** is a consequence of [CV86]. Continuous dependence on ω for some examples was proved in [Gua08].

Assumption **(3)** is reminiscent of what usually appears in the case of the non-linear Schrödinger equations, see [Wei85; Wei86; SS85; GSS87]. This goes back to Vakhitov and Kolokolov [VK73].

The space of functions satisfying **(4)** is invariant by (NLDE). Since we imposed $3\omega > m$, we have that $\pm 2i\omega$ are embedded eigenvalues. We can avoid this thanks to the symmetry **(4)** since the associated eigenvectors do not belong to $\mathbf{X}$. Reducing to the space $\mathbf{X}$ reduces the number of parameters, simplifying the problem. The parameters eliminated involve translation and orientation of the solutions.

Assumption **(5)** has to be linked to Definition 7.3 and the Krein signature in Theorem 7.6. The first link is natural as Jordan blocks (outside the natural one for the kernel) will produce linear instability. The second link shows that instability cannot occur by modulating ω.

By **(6)**–**(8)** there are no resonances for the restriction of $i\mathbf{L}(\omega)$ in $\mathbf{X}$. As expected, **(8)** had been verified in [BC12b].

The assumptions **(7)**, **(10)**, **(11)** and **(12)** are considered as generic in the sense that they are not true for some g a small change will change the situation. Surprisingly, no proof of such statement seems available.

The most technical assumption is **(12)**, we actually rewrote the original one, the one presented is stronger. The reason is that the original assumptions reads only on a coordinate system that we obtained after several changes changes of variables that are maybe useless to present here. Note that actually these changes of variables are small perturbations of the identity so that replacing them by the identity gives the current form of **(12)** out of the original one. One interest of the form we gave here, is that it is closer to the usual formulation of the Fermi Golden Rule in the semi-linear context. One motivation of our original formulation is that even if **(12)** is not satisfied the Fermi Golden Rule in [BC12c] could be. Another motivation is that formulated in an appropriate hamiltonian framework we hope that this formulation may turn to be in some convenient form to analyse the dynamics.

A restrictive assumption is actually **(5)** as it imposes to the point spectrum to be semi-simple with non-zero Krein signature. This last requirement is compatible with the considerations of the previous section on the spectral stability.

We finish this paragraph by mentioning that we introduced the charge conjugation C to replace the usual complex conjugation. The standard Dirac operator commutes to C but not to the complex conjugation. For the usual complex conjugation, the linearisation writes in splitting real and imaginary parts. The same can be done with the charge conjugation with the corresponding real and imaginary parts. For the hamiltonian consideration mentioned below this is more convenient.

A linear combination will change one splitting to the other and the matrix Σ_3 that appears in the assumptions is actually the J matrix of the previous section written in the coordinates associated to the charge conjugation splitting.

7.2.2 The asymptotic stability

The main result of our analysis is the

Theorem 7.8. *Suppose that $\mathcal{O} \subset (m/3, m)$ and fix $k_0 \geq 4$, $k_0 \in \mathbb{Z}$. Pick $\omega_1 \in \mathcal{O}$ and let $\phi_{\omega_0}(x)$ be a standing wave of (NLDE). Let $u(t,x)$ be a solution to (NLDE). Assume* **(1)–(12)** *(at ω_0). Then, there exist an $\epsilon_0 > 0$ and a $C > 0$ such that for any $\epsilon \in (0, \epsilon_0)$ and for any u_0 with $\inf_{\gamma\in\mathbb{R}} \|u_0 - e^{i\gamma}\phi_{\omega_1}\|_{H^{k_0}} < \epsilon$, there exist $\omega_+ \in \mathcal{O}$, $\theta \in C^1(\mathbb{R};\mathbb{R})$ and $h_+ \in H^{k_0}$ with $\|h_+\|_{H^{k_0}} + |\omega_+ - \omega_0| \leq C\epsilon$ such that*

$$\lim_{t\to+\infty} \|u(t,\cdot) - e^{i\theta(t)}\phi_{\omega_+} - e^{-itD_m}h_+\|_{H^{k_0}} = 0.$$

The constraint $3\omega > m$ allows to exploit the non-linear Fermi Golden Rule like for the non-linear Schrödinger equation by circumventing the strong indefiniteness of the Dirac system. This guarantees that appropriate multiples of the eigenvalues belong to portions of the spectrum where there is no superposition of the continuous spectrum of distinct coordinates. This fact and our results continue to hold if $3\omega < m$ and $(2N_j + 1)\omega > m$ for all $j = 1, ..., n$.

It is still difficult to provide examples of g and ω satisfying our spectral assumptions. The situation is not very different from the case of the NLS where the spectrum is unknown except in few cases. Rigorous analysis of examples is certainly a difficult open problem. Like for the NLS, see [Cha+08], one can consider numerical analysis.

We refer to Section 7.1 for an account of what is known for the Dirac equation. These are ongoing works and we expect to attain a situation which can be almost as satisfactory as in the Schrödinger case.

Consider $\xi \in \mathrm{Ker}(\mathcal{H}_\omega - \lambda_j(\omega))$. One of the requirements for linear stability in Definition 7.7 is that if $\xi \neq 0$ then $\langle \xi, \Sigma_3\xi^* \rangle > 0$. As it might seem artificial, we stated the

Theorem 7.9. *Suppose that $\mathcal{O} \subset (m/3, m)$. Pick $\omega \in \mathcal{O}$ and let $\phi_\omega(x)$ be a standing wave of (NLDE). Replace* **(5)** *with the following assumption:*

(H:5') *We assume that $i\mathbf{L}(\omega)$ satisfies all the conditions of Definition 7.7 except for condition (4) which we restate as follows. That is, we assume that for any eigenvalue $\lambda > 0$ the quadratic form $\xi \to \langle \xi, \Sigma_3\xi^* \rangle$ is non degenerate in $\mathrm{Ker}(i\mathbf{L}(\omega) - \lambda)$. We assume that there exists at least one eigenvalue $\lambda > 0$ such that the quadratic form is non positive in $\mathrm{Ker}(i\mathbf{L}(\omega) - \lambda)$.*

Assume **(1)–(4)**, **(H:5')** *and* **(6)–(12)**. *Then $\phi_\omega(x)$ is orbitally unstable.*

This instability result in Theorem 7.9 arose from our desire to justify Assumption **(5)** in our definition of linear stability, see Definition 7.7.

The strategy of our proofs began with a classical linear analysis where we considered the linearisation of (NLDE) at the stationary solution, and gave some information on the spectrum and on symmetries of the linearisation.

We introduced an appropriate coordinate system related to the spectral decomposition of the linearised operator. We especially insisted in having a hamiltonian formulation of the problem in terms of the coordinates. Except for the dispersive part all the coordinates go in pairs of conjugate coordinates. This is for instance why we considered the pair (z, Cz) in a way similar to the scalar case. The system was rewritten in a hamiltonian form, as we wanted to use some of the machinery used in the stability analysis of finite dimensional hamiltonian systems. Unfortunately for the natural sympleptic structure of the system, $\langle X, \mathrm{i}Y\rangle$, the coordinates were not canonical. So by means of a Darboux theorem of our own, we changed variables to canonical coordinates. We then applied the method of Birkhoff normal forms to isolate key resonating terms and prove non-linear dispersion. The key being the Fermi Golden Rule **(12)**.

Specifically we proved that appropriate coefficients are quadratic forms and that for $\omega > m/3$ they are non negative and under hypothesis **(12)** they are nonzero. Then using some of the linear theory of dispersion in [Bou06; Bou08] we obtained the stability.

7.3 An ongoing work: The non-relativistic limit

The result presented so far are quite restrictive in the sense that they are conditional to the knowledge of what is the spectrum of some limit operator.

In a work in progress with Andrew Comech [BC], we consider the limit as ω tends to $\pm m$ which corresponds to the non-relativistic limit.

We built particular families of solitary wave solutions to the non-linear Dirac equation (NLDE) which "bifurcate" from solitary waves of its non-relativistic limit, the non-linear Schrödinger equation (NLS). In [Gua08] or [CGG14] such a bifurcation was obtained by means of an implicit function theorem. They thus assumed that the non-linearity g is smooth enough. So the non-relativistic limit is a mass super-critical non-linear Schrödinger equation and thus the corresponding ground state is unstable. To recover stable limits, we use a Shauder fixed point argument coupled to shooting type arguments to obtain the

Theorem 7.10. *Let $n \in \mathbb{N}$. Assume that*

$$g(s) = |s|^k + O(|s|^K), \qquad 0 < k < K.$$

If $n \geq 3$, additionally assume that $k < 2/(n-2)$. There is $\omega_0 < m$, dependent on n and g, such that for $\omega \in (\omega_0, m)$ there are solutions ϕ_ω to

$$\omega\phi_\omega = D_m\phi_\omega - g(\phi_\omega^*\beta\phi_\omega)\beta\phi_\omega,$$

so that $\phi_\omega(x)e^{-\mathrm{i}\omega t}$ is a solitary wave solution to (NLDE), and

$$\phi_\omega(x)^*\beta\phi_\omega(x) \geq |\phi_\omega(x)|^2/2, \qquad x \in \mathbb{R}^n. \tag{7.8}$$

Moreover, introducing the projections onto the "particle" and "antiparticle" components,

$$\mathit{\Pi}_P = \frac{1}{2}(1+\beta), \qquad \mathit{\Pi}_A = \frac{1}{2}(1-\beta); \qquad \phi_P(x) = \mathit{\Pi}_P\phi(x), \qquad \phi_A(x) = \mathit{\Pi}_A\phi(x),$$

we have for $\epsilon = \sqrt{m^2 - \omega^2}$ *and some* $\tau > 0$*:*

$$\|e^{\tau\langle Q\rangle}(\phi_P - \epsilon^{\frac{1}{k}}\hat{\Phi}_P(\epsilon\cdot))\|_{H^1\cap L^\infty} = O(\epsilon^{2\min(1,k,\frac{K}{k}-1)+\frac{1}{k}}),$$

$$\|e^{\tau\langle Q\rangle}(\phi_A - \epsilon^{1+\frac{1}{k}}\hat{\Phi}_A(\epsilon\cdot))\|_{H^1\cap L^\infty} = O(\epsilon^{1+2\min(1,k,\frac{K}{k}-1)+\frac{1}{k}}),$$

where

$$\hat{\Phi}_P(y) = \boldsymbol{n}u_k(y), \qquad \hat{\Phi}_A = -\frac{\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\hat{\Phi}_P}{2m},$$

with $\boldsymbol{n} \in \mathbb{C}^N$, $|\boldsymbol{n}| = 1$, $\Pi_P\boldsymbol{n} = \boldsymbol{n}$, *and* $u_k \in H^s(\mathbb{R}^n, \mathbb{R})$, $s = [(n+3)/2]$, *a strictly positive spherically symmetric solution to*

$$-\frac{1}{2m}u = -\frac{1}{2m}\Delta u - |u|^{2k}u, \qquad u(x) \in \mathbb{R}, \quad x \in \mathbb{R}^n.$$

The property (7.8) is crucial to the spectral stability analysis to ensure the Fréchet differentiability of the non-linear term (outside 0). This is actually for this property that we used shooting type arguments

From the above theorem, one can wonder if the non-relativistic limit holds at the level of the linearisation. The next theorem we obtain is still a the general level and aimed at giving the asymptotic of the spectrum. This was the first step towards a refinement of Theorem 7.6.

Theorem 7.11 (Bifurcation of point eigenvalues from the spectrum of the free Dirac operator)**.** *Let* $n \geq 1$. *Let* $J \in \mathrm{End}\,(\mathbb{C}^N)$ *be skew-adjoint and invertible,* $\sigma(J) = \{\pm\mathrm{i}\}$, $[J, D_m] = 0$. *Let* $(\omega_j)_{j\in\mathbb{N}}$, $\omega_j \in \mathcal{O}$, *be a Cauchy sequence,* $\omega_j \to \omega_b = \pm m$, *and assume that there is* $\varepsilon > 0$ *such that*

$$\lim_{j\to\infty} \left\|\langle Q\rangle^{1+\varepsilon}V(\omega_j)\right\|_{L^\infty(\mathbb{R}^n,\,\mathrm{End}\,(\mathbb{C}^N))} = 0.$$

Let $\lambda_j \in \sigma_{\mathrm{p}}(JL(\omega_j))$, *and let* $\lambda_b \in \mathrm{i}\mathbb{R}\cup\{\infty\}$ *be an accumulation point of the sequence* $(\lambda_j)_{j\in\mathbb{N}}$. *Then:*

1. $\lambda_b \in \{0; \pm 2m\mathrm{i}\}$. *In particular,* $\lambda_b \neq \infty$.
2. *If additionally* $\Re\lambda_j \neq 0$ *and* $\lambda_j \to \lambda_b = 0$, *then* $\lambda_j = O(m^2 - \omega_j^2)$.

We relate the families of eigenvalues of the linearised non-linear Dirac equation bifurcating from $\lambda = 0$ with the eigenvalues of the linearised non-linear Schrödinger equation (NLS). Let $n \leq 3$. By [BL83, Example 1], the equation

$$-\frac{1}{2m}u = -\frac{1}{2m}\Delta u - |u|^{2k}u, \qquad u(x) \in \mathbb{R}, \quad x \in \mathbb{R}^n$$

has a strictly positive spherically symmetric exponentially decaying solution $u_k(x)$ if and only if $0 < k < 2/(n-2)$ (any $k > 0$ if $n \leq 2$). It follows that $u_k(x)e^{-\mathrm{i}\omega t}$ with $\omega = -\frac{1}{2m}$ is a solitary wave solution to (NLS). The linearisation at this solitary wave, see Section 7.1.2, is given by $\mathbf{jl}(\omega)$. *In fine*, we can prove the

Theorem 7.12 (Bifurcations from the origin at $\omega = m$)**.** *Let* $n \geq 1$ *and* $0 < k < K$. *If* $n \geq 3$, *additionally assume that* $k < 2/(n-2)$. *Let* $g(s) = |s|^k + O(|s|^K)$. *Let* $\omega_j \to m$ *and let* $\phi_{\omega_j}e^{-\mathrm{i}\omega_j t}$ *be a family of solitary wave solutions to* (NLDE) *constructed in Theorem 7.10 below. Assume that* λ_j *are eigenvalues of* (NLDE) *linearised at* $\phi_{\omega_j}e^{-\mathrm{i}\omega_j t}$ *such that*

$$\Re\lambda_j \neq 0, \qquad \lambda_j = O(m^2 - \omega_j^2)$$

(cf. Theorem 7.11 1), and denote

$$\Lambda_j := \frac{\lambda_j}{m^2 - \omega_j^2}.$$

1. *If Λ_b is an accumulation point of the sequence $(\Lambda_j)_{j\in\mathbb{N}}$, then $\Lambda_b \in \sigma_{\mathrm{p}}(\mathbf{j}\mathfrak{l})$.*

2. *If, moreover,*

$$\sigma_{\mathrm{p}}(\mathbf{j}\mathfrak{l}) \cap \sigma_{\mathrm{p}}(-\mathrm{i}\mathfrak{l}_-) = \{0\}, \qquad \sigma_{\mathrm{p}}(\mathbf{j}\mathfrak{l}) \cap \sigma_{\mathrm{p}}(\mathrm{i}\mathfrak{l}_-) = \{0\},$$

   then $\Lambda_b \in \sigma_{\mathrm{p}}(\mathbf{j}\mathfrak{l}) \cap \mathbb{R}$.

3. *If $\lambda_j \neq 0$ for $j \in \mathbb{N}$, then $\Lambda_b = 0$ is only possible when $k = \frac{2}{n}$.*

4. *If $\Re\lambda_j \neq 0$ for $j \in \mathbb{N}$, then $\Lambda_b = 0$ is only possible when $k = \frac{2}{n}$ and $\partial_\omega Q(\phi_\omega) > 0$ for $\omega \in (\omega_0, m)$, with some $\omega_0 < m$. Moreover, $\Im\lambda_j = 0$ for all but finitely many $j \in \mathbb{N}$.*

This theorem reduces our initial problem to a well known case, the one of the non-linear Schrödinger equation. Unfortunately, this case is far from being completely solved. For instance, in the analysis [Cha+08] the authors have to complement their partial theoretical results by numerical evidences. In [CHS12], the authors proved the gap condition ($\ell(\omega)$ and $\ell^-(\omega)$ has no eigenvalues in $(0, \omega]$ among other things) only in dimension 3 for the cubic case ($k = 1/2$) restricted to the radial symmetric solutions.

References

[BC] N. Boussaïd and A. Comech. “ Linear stability of the nonlinear Dirac equation in the nonrelativistic limit ”.

[BC12a] G. Berkolaiko and A. Comech. “ On spectral stability of solitary waves of nonlinear Dirac equation in 1D ” . In: *Math. Model. Nat. Phenom.* 7.2 (2012), pp. 13–31. DOI: 10.1051/mmnp/20127202. URL: http://dx.doi.org/10.1051/mmnp/20127202.

[BC12b] N. Boussaïd and A. Comech. *On spectral stability of the nonlinear Dirac equation.* 2012. arXiv: 1211.3336 [math.AP].

[BC12c] N. Boussaïd and S. Cuccagna. “ On stability of standing waves of nonlinear Dirac equations ” . In: *Comm. Partial Differential Equations* 37.6 (2012), pp. 1001–1056. DOI: 10.1080/03605302.2012.665973. URL: http://hal.archives-ouvertes.fr/hal-00578790/PDF/StabDirac20120103.pdf.

[BG87] A. Berthier and V. Georgescu. “ On the point spectrum of Dirac operators ” . In: *J. Funct. Anal.* 71.2 (1987), pp. 309–338. DOI: 10.1016/0022-1236(87)90007-3. URL: http://dx.doi.org/10.1016/0022-1236(87)90007-3.

[BL83] H. Berestycki and P.-L. Lions. “ Nonlinear scalar field equations. I. Existence of a ground state ” . In: *Arch. Rational Mech. Anal.* 82.4 (1983), pp. 313–345. DOI: 10.1007/BF00250555. URL: http://dx.doi.org/10.1007/BF00250555.

[Bou06] N. Boussaïd. “ Stable directions for small nonlinear Dirac standing waves ” . In: *Comm. Math. Phys.* 268.3 (2006), pp. 757–817. DOI: 10.1007/s00220-006-0112-3. URL: http://hal.archives-ouvertes.fr/hal-00016041/PDF/Article-StabilizationSmallDirac%20SolitonNonResonantCaseFinal.pdf.

[Bou08] N. Boussaïd. " On the asymptotic stability of small nonlinear Dirac standing waves in a resonant case " . In: *SIAM J. Math. Anal.* 40.4 (2008), pp. 1621–1670. DOI: 10.1137/070684641. URL: http://hal.archives-ouvertes.fr/hal-00116269/PDF/Article-2-StabilizationSmallDir%20acSolitonResonantCaseFinal41.pdf.

[CGG14] A. Comech, M. Guan, and S. Gustafson. " On linear instability of solitary waves for the nonlinear Dirac equation " . In: *Ann. Inst. H. Poincaré Anal. Non Linéaire* 31.3 (2014), pp. 639–654. DOI: 10.1016/j.anihpc.2013.06.001. URL: http://dx.doi.org/10.1016/j.anihpc.2013.06.001.

[Cha+08] S.-M. Chang, S. Gustafson, K. Nakanishi, and T.-P. Tsai. " Spectra of linearized operators for NLS solitary waves " . In: *SIAM J. Math. Anal.* 39.4 (2007/08), pp. 1070–1111. DOI: 10.1137/050648389. URL: http://dx.doi.org/10.1137/050648389.

[CHS12] O. Costin, M. Huang, and W. Schlag. " On the spectral properties of $L_\pm$ in three dimensions " . In: *Nonlinearity* 25 (Jan. 2012), pp. 125–164. DOI: 10.1088/0951-7715/25/1/125. arXiv: 1107.0323 [math.AP].

[CL82] T. Cazenave and P.-L. Lions. " Orbital stability of standing waves for some nonlinear Schrödinger equations ". In: *Comm. Math. Phys.* 85.4 (1982), pp. 549–561. URL: http://projecteuclid.org/euclid.cmp/1103921547.

[CV86] T. Cazenave and L. Vázquez. " Existence of localized solutions for a classical nonlinear Dirac field ". In: *Comm. Math. Phys.* 105.1 (1986), pp. 35–47. URL: http://projecteuclid.org/euclid.cmp/1104115255.

[GSS87] M. Grillakis, J. Shatah, and W. Strauss. " Stability theory of solitary waves in the presence of symmetry. I " . In: *J. Funct. Anal.* 74.1 (1987), pp. 160–197. DOI: 10.1016/0022-1236(87)90044-9. URL: http://dx.doi.org/10.1016/0022-1236(87)90044-9.

[Gua08] M. Guan. " Solitary Wave Solutions for the Nonlinear Dirac Equations ". In: *ArXiv e-prints* (Dec. 2008). arXiv: 0812.2273 [math.AP].

[SS85] J. Shatah and W. Strauss. " Instability of nonlinear bound states ". In: *Comm. Math. Phys.* 100.2 (1985), pp. 173–190.

[Tha92] B. Thaller. *The Dirac equation*. Texts and Monographs in Physics. Berlin, 1992, pp. xviii+357. DOI: 10.1007/978-3-662-02753-0. URL: http://dx.doi.org/10.1007/978-3-662-02753-0.

[VK73] N. G. Vakhitov and A. A. Kolokolov. " Stationary solutions of the wave equation in the medium with nonlinearity saturation " . In: *Radiophys. Quantum Electron.* 16 (1973), pp. 783–789. DOI: 10.1007/BF01031343.

[Wei85] M. I. Weinstein. " Modulational stability of ground states of nonlinear Schrödinger equations ". In: *SIAM J. Math. Anal.* 16.3 (1985), pp. 472–491.

[Wei86] M. I. Weinstein. " Lyapunov stability of ground states of nonlinear dispersive evolution equations ". In: *Comm. Pure Appl. Math.* 39.1 (1986), pp. 51–67.

Part IV

Bibliography

List of publications

[BB10] L. Boulton and N. Boussaïd. " Non-variational computation of the eigenstates of Dirac operators with radially symmetric potentials " . In: *LMS J. Comput. Math.* 13 (2010), pp. 10–32. DOI: 10.1112/S1461157008000429. URL: http://hal.archives-ouvertes.fr/hal-00308843/PDF/Preprint-DiracNumerical.pdf.

[BBBa] G. R. Barrenechea, L. Boulton, and N. Boussaïd. *Eigenvalue enclosures*. URL: http://hal.archives-ouvertes.fr/hal-00837475.

[BBBb] G. R. Barrenechea, L. Boulton, and N. Boussaïd. *Finite element eigenvalue enclosures for the Maxwell operator*. URL: http://hal.archives-ouvertes.fr/hal-00949589.

[BBL12] L. Boulton, N. Boussaïd, and M. Lewin. " Generalised Weyl theorems and spectral pollution in the Galerkin method " . In: *J. Spectr. Theory* 2.4 (2012), pp. 329–354. DOI: 10.4171/JST/32. URL: http://hal.archives-ouvertes.fr/hal-00536270/PDF/Weyl32.pdf.

[BC12a] N. Boussaïd and A. Comech. *On spectral stability of the nonlinear Dirac equation*. 2012. arXiv: 1211.3336 [math.AP].

[BC12b] N. Boussaïd and S. Cuccagna. " On stability of standing waves of nonlinear Dirac equations " . In: *Comm. Partial Differential Equations* 37.6 (2012), pp. 1001–1056. DOI: 10.1080/03605302.2012.665973. URL: http://hal.archives-ouvertes.fr/hal-00578790/PDF/StabDirac20120103.pdf.

[BCC12a] N. Boussaïd, M. Caponigro, and T. Chambrion. " Approximate controllability of the Schrödinger equation with a polarizability term " . In: *Decision and Control (CDC), 2012 IEEE 51st Annual Conference on*. IEEE. 2012, pp. 3024–3029. DOI: 10.1109/CDC.2012.6426619. URL: http://hal.archives-ouvertes.fr/hal-00784881/PDF/Quadratique13.pdf.

[BCC12b] N. Boussaïd, M. Caponigro, and T. Chambrion. " Implementation of logical gates on infinite dimensional quantum oscillators ". In: *American Control Conference (ACC), 2012*. IEEE. 2012, pp. 5825–5830. URL: http://hal.archives-ouvertes.fr/hal-00637115/PDF/QG%5C_ACC%5C_0.6.pdf.

[BCC12c] N. Boussaïd, M. Caponigro, and T. Chambrion. " Periodic control laws for bilinear quantum systems with discrete spectrum ". In: *American Control Conference (ACC), 2012*. IEEE. 2012, pp. 5819–5824. URL: http://hal.archives-ouvertes.fr/hal-00637116/PDF/FEPS%5C_ACC%5C_3.pdf.

[BCC12d] N. Boussaïd, M. Caponigro, and T. Chambrion. " Small time reachable set of bilinear quantum systems " . In: *Decision and Control (CDC), 2012 IEEE 51st Annual Conference on*. IEEE. 2012, pp. 1083–1087. DOI: 10.1109/CDC.2012.6426208. URL: http://hal.archives-ouvertes.fr/hal-00710040/PDF/Time06.pdf.

[BCC12e] N. Boussaïd, M. Caponigro, and T. Chambrion. " Which notion of energy for bilinear quantum systems? " In: *proceeding of the 4th IFAC Workshop on Lagrangian and Hamiltonian Methods for Non Linear Control, pp 226-230, 29-31 août 2012*. 2012, pp. 226–230. DOI: 10.3182/20120829-3-IT-4022.00034. URL: http://hal.archives-ouvertes.fr/hal-00784890/PDF/Energy4.pdf.

[BCC13a] N. Boussaïd, M. Caponigro, and T. Chambrion. " Energy Estimates for Low Regularity Bilinear Schrödinger Equations " . In: *Control of Systems Governed by Partial Differential Equations*. Vol. 1. 1. 2013, pp. 25–30. DOI: 10.3182/20130925-3-FR-4043.00046. URL: http://hal.archives-ouvertes.fr/hal-00784876/PDF/cpde09.pdf.

[BCC13b] N. Boussaïd, M. Caponigro, and T. Chambrion. " Total variation of the control and energy of bilinear quantum systems " . In: *Decision and Control (CDC), 2013 IEEE 52nd Annual Conference on*. Dec. 2013, pp. 3714–3719. DOI: 10.1109/CDC.2013.6760455. URL: http://hal.archives-ouvertes.fr/hal-00800548/PDF/BVefficiency09.pdf.

[BCC13c] N. Boussaïd, M. Caponigro, and T. Chambrion. " Weakly coupled systems in quantum control " . In: *IEEE Trans. Automat. Control* 58.9 (2013), pp. 2205–2216. DOI: 10.1109/TAC.2013.2255948.

[BCC14a] N. Boussaïd, M. Caponigro, and T. Chambrion. *Approximate controllability of the Schrödinger Equation with a polarizability term in higher Sobolev norms*. June 2014. URL: http://hal.archives-ouvertes.fr/hal-01006178.

[BCC14b] N. Boussaïd, M. Caponigro, and T. Chambrion. *Efficient finite dimensional approximations for the bilinear Schrodinger equation with bounded variation controls*. 2014. URL: http://hal.archives-ouvertes.fr/hal-01003056.

[BCC14c] N. Boussaïd, M. Caponigro, and T. Chambrion. *Regular propagators of bilinear quantum systems*. June 2014. URL: http://hal.archives-ouvertes.fr/hal-01016299.

[BDF11] N. Boussaïd, P. D'Ancona, and L. Fanelli. " Virial identity and weak dispersion for the magnetic Dirac equation " . In: *J. Math. Pures Appl. (9)* 95.2 (2011), pp. 137–150. DOI: 10.1016/j.matpur.2010.10.004. URL: http://hal.archives-ouvertes.fr/hal-00430346/PDF/diracsmoo-20091218.pdf.

[BG10] N. Boussaïd and S. Golénia. " Limiting absorption principle for some long range perturbations of Dirac systems at threshold energies " . In: *Comm. Math. Phys.* 299.3 (2010), pp. 677–708. DOI: 10.1007/s00220-010-1099-3. URL: http://hal.archives-ouvertes.fr/hal-00392422/PDF/LAPDLRvHAL20090608.pdf.

[Bou06a] N. Boussaïd. "Étude de la stabilité des petites solutions stationnaires pour une classe déquations de Dirac non linéaires". July 2006. URL: http://tel.archives-ouvertes.fr/tel-00108459/PDF/These.pdf.

[Bou06b] N. Boussaïd. " Stable directions for small nonlinear Dirac standing waves " . In: *Comm. Math. Phys.* 268.3 (2006), pp. 757–817. DOI: 10.1007/s00220-006-0112-3. URL: http://hal.archives-ouvertes.fr/hal-00016041/PDF/Article-StabilizationSmallDirac%20SolitonNonResonantCaseFinal.pdf.

[Bou07] N. Boussaïd. *A stability result for small stationary solutions of a class of nonlinear Dirac equations*. 2007. URL: http://basepub.dauphine.fr/xmlui/handle/123456789/6543.

[Bou08] N. Boussaïd. " On the asymptotic stability of small nonlinear Dirac standing waves in a resonant case " . In: *SIAM J. Math. Anal.* 40.4 (2008), pp. 1621–1670. DOI: 10.1137/070684641. URL: http://hal.archives-ouvertes.fr/hal-00116269/PDF/Article-2-StabilizationSmallDir%20acSolitonResonantCaseFinal41.pdf.

References of Chapter 2

[ABG96] W. O. Amrein, A. Boutet de Monvel, and V. Georgescu. *C_0-groups, commutator methods and spectral theory of N-body Hamiltonians*. Vol. 135. Progress in Mathematics. Basel, 1996, pp. xiv+460.

[Amr+98] C. Amrouche, C. Bernardi, M. Dauge, and V. Girault. " Vector potentials in three-dimensional non-smooth domains ". In: *Math. Methods Appl. Sci.* 21.9 (1998), pp. 823–864.

[AY82] M. Arai and O. Yamada. " Essential selfadjointness and invariance of the essential spectrum for Dirac operators " . In: *Publ. Res. Inst. Math. Sci.* 18.3 (1982), pp. 973–985. DOI: 10.2977/prims/1195183289. URL: http://dx.doi.org/10.2977/prims/1195183289.

[BC12] N. Boussaïd and A. Comech. *On spectral stability of the nonlinear Dirac equation*. 2012. arXiv: 1211.3336 [math.AP].

[BM97] A. Boutet de Monvel and M. Măntoiu. *The method of the weakly conjugate operator*. Apagyi, Barnabás (ed.) et al., Inverse and algebraic quantum scattering theory. Proceedings of a conference, held at Lake Balaton, Hungary. 3–7 September 1996. Berlin: Springer. Lect. Notes Phys. 488, 204-226 (1997). 1997.

[BS90] M. Birman and M. Solomyak. " The self-adjoint Maxwell operator in arbitrary domains ". In: *Leningrad Math. J* 1.1 (1990), pp. 99–115.

[Che77] P. R. Chernoff. " Schrödinger and Dirac operators with singular potentials and hyperbolic equations ". In: *Pacific J. Math.* 72.2 (1977), pp. 361–382.

[Dir28] P. A. M. Dirac. " The Quantum Theory of the Electron " . In: *Royal Society of London Proceedings Series A* 117 (Feb. 1928), pp. 610–624. DOI: 10.1098/rspa.1928.0023.

[EL07] M. Esteban and M. Loss. " Self-adjointness for Dirac operators via Hardy-Dirac inequalities ". In: *J. Math. Phys.* 48.11 (2007), pp. 112107, 8.

[Gér08] C. Gérard. " A proof of the abstract limiting absorption principle by energy estimates " . In: *J. Funct. Anal.* 254.11 (2008), pp. 2707–2724. DOI: 10.1016/j.jfa.2008.02.015. URL: http://dx.doi.org/10.1016/j.jfa.2008.02.015.

[GGM04] V. Georgescu, C. Gérard, and J. S. Møller. " Commutators, C_0-semigroups and resolvent estimates ". In: *J. Funct. Anal.* 216.2 (2004), pp. 303–361.

[GJ07] S. Golénia and T. Jecko. " A new look at Mourre's commutator theory. " In: *Complex Anal. Oper. Theory* 1.3 (2007), pp. 399–422.

[GR86] V. Girault and P.-A. Raviart. *Finite element methods for Navier-Stokes equations*. Vol. 5. Springer Series in Computational Mathematics. Theory and algorithms. Berlin, 1986, pp. x+374.

[IM99] A. Iftimovici and M. Măntoiu. " Limiting absorption principle at critical values for the Dirac operator ". In: *Lett. Math. Phys.* 49.3 (1999), pp. 235–243.

[Kal98] H. Kalf. " Essential self-adjointness of Dirac operators under an integral condition on the potential " . In: *Lett. Math. Phys.* 44.3 (1998), pp. 225–232. DOI: 10.1023/A:1007415716921. URL: http://dx.doi.org/10.1023/A:1007415716921.

[Kat66] T. Kato. “ Wave operators and similarity for some non-selfadjoint operators ”. In: *Math. Ann.* 162 (1965/1966), pp. 258–279.

[Kes61] H. Kestelman. “ Anticommuting linear transformations ”. In: *Canad. J. Math.* 13 (1961), pp. 614–624.

[Kla80] M. Klaus. “ Dirac operators with several Coulomb singularities ”. In: *Helv. Phys. Acta* 53.3 (1980), 463–482 (1981).

[KY01] H. Kalf and O. Yamada. “ Essential self-adjointness of n-dimensional Dirac operators with a variable mass term ” . In: *J. Math. Phys.* 42.6 (2001), pp. 2667–2676. DOI: 10.1063/1.1367331. URL: http://dx.doi.org/10.1063/1.1367331.

[KY89] T. Kato and K. Yajima. “ Some examples of smooth operators and the associated smoothing effect ” . In: *Rev. Math. Phys.* 1.4 (1989), pp. 481–496. DOI: 10.1142/S0129055X89000171. URL: http://dx.doi.org/10.1142/S0129055X89000171.

[LO77] B. M. Levitan and M. Otelbaev. “ Conditions for the selfadjointness of Schrödinger and Dirac operators ”. In: *Dokl. Akad. Nauk SSSR* 235.4 (1977), pp. 768–771.

[LR79] J. J. Landgren and P. A. Rejto. “ An application of the maximum principle to the study of essential selfadjointness of Dirac operators. I ” . In: *J. Math. Phys.* 20.11 (1979), pp. 2204–2211. DOI: 10.1063/1.523999. URL: http://dx.doi.org/10.1063/1.523999.

[LRK80] J. J. Landgren, P. A. Rejto, and M. Klaus. “ An application of the maximum principle to the study of essential selfadjointness of Dirac operators. II ” . In: *J. Math. Phys.* 21.5 (1980), pp. 1210–1217. DOI: 10.1063/1.524546. URL: http://dx.doi.org/10.1063/1.524546.

[Mou81] E. Mourre. “ Absence of singular continuous spectrum for certain selfadjoint operators ”. In: *Comm. Math. Phys.* 78.3 (1980/81), pp. 391–408. URL: http://projecteuclid.org/euclid.cmp/1103908694.

[Nen75] G. Nenciu. “ Eigenfunction expansions for Schrödinger and Dirac operators with singular potentials ”. In: *Comm. Math. Phys.* 42 (1975), pp. 221–229.

[Pau36] W. Pauli. “ Contributions mathématiques à la théorie des matrices de Dirac ”. In: *Ann. Inst. H. Poincaré* 6.2 (1936), pp. 109–136. URL: http://www.numdam.org/item?id=AIHP_1936__6_2_109_0.

[Put67] C. R. Putnam. *Commutation properties of Hilbert space operators and related topics.* Ergebnisse der Mathematik und ihrer Grenzgebiete, Band 36. 1967, pp. xi+167.

[Ran] A. F. Ranada. “Classical nonlinear Dirac field models of extended particles”. In: *Quantum theory, groups, fields and particles,* vol. 198. Amsterdam, Reidel, pp. 271–291.

[RS04] I. Rodnianski and W. Schlag. “ Time decay for solutions of Schrödinger equations with rough and time-dependent potentials ” . In: *Invent. Math.* 155.3 (2004), pp. 451–513. DOI: 10.1007/s00222-003-0325-4. URL: http://dx.doi.org/10.1007/s00222-003-0325-4.

[RS78] M. Reed and B. Simon. *Methods of modern mathematical physics. IV. Analysis of operators.* New York, 1978, pp. xv+396.

[RS79] M. Reed and B. Simon. *Methods of modern mathematical physics. III.* Scattering theory. 1979, pp. xv+463.

[RS80] M. Reed and B. Simon. *Methods of modern mathematical physics. I.* Second. Functional analysis. New York, 1980, pp. xv+400.

[Shi11] D. S. Shirokov. " Extension of Pauli's theorem to the case of Clifford algebras " . In: *Dokl. Akad. Nauk* 440.5 (2011), pp. 607–610. DOI: 10.1134/S1064562411060329. URL: http://dx.doi.org/10.1134/S1064562411060329.

[Shi13] D. Shirokov. " Pauli theorem in the description of n-dimensional spinors in the Clifford algebra formalism " . In: *Theoretical and Mathematical Physics* 175.1 (2013), pp. 454–474. DOI: 10.1007/s11232-013-0038-9. URL: http://dx.doi.org/10.1007/s11232-013-0038-9.

[Tha92] B. Thaller. *The Dirac equation*. Texts and Monographs in Physics. Berlin, 1992, pp. xviii+357. DOI: 10.1007/978-3-662-02753-0. URL: http://dx.doi.org/10.1007/978-3-662-02753-0.

[Wae74] B. L. van der Waerden. *Group theory and quantum mechanics*. Translated from the 1932 German original, Die Grundlehren der mathematischen Wissenschaften, Band 214. New York, 1974, pp. viii+211.

[Xia99] J. Xia. " On the contribution of the Coulomb singularity of arbitrary charge to the Dirac Hamiltonian " . In: *Trans. Amer. Math. Soc.* 351.5 (1999), pp. 1989–2023. DOI: 10.1090/S0002-9947-99-02084-X. URL: http://dx.doi.org/10.1090/S0002-9947-99-02084-X.

References of Part II

[Bou06a] N. Boussaïd. "Étude de la stabilité des petites solutions stationnaires pour une classe déquations de Dirac non linéaires". July 2006. URL: http://tel.archives-ouvertes.fr/tel-00108459/PDF/These.pdf.

[Bou06b] N. Boussaïd. " Stable directions for small nonlinear Dirac standing waves " . In: *Comm. Math. Phys.* 268.3 (2006), pp. 757–817. DOI: 10.1007/s00220-006-0112-3. URL: http://hal.archives-ouvertes.fr/hal-00016041/PDF/Article-StabilizationSmallDirac%20SolitonNonResonantCaseFinal.pdf.

[Bou07] N. Boussaïd. *A stability result for small stationary solutions of a class of nonlinear Dirac equations*. 2007. URL: http://basepub.dauphine.fr/xmlui/handle/123456789/6543.

[Bou08] N. Boussaïd. " On the asymptotic stability of small nonlinear Dirac standing waves in a resonant case " . In: *SIAM J. Math. Anal.* 40.4 (2008), pp. 1621–1670. DOI: 10.1137/070684641. URL: http://hal.archives-ouvertes.fr/hal-00116269/PDF/Article-2-StabilizationSmallDir%20acSolitonResonantCaseFinal41.pdf.

[JK79] A. Jensen and T. Kato. " Spectral properties of Schrödinger operators and time-decay of the wave functions ". In: *Duke Math. J.* 46.3 (1979), pp. 583–611.

[KT98] M. Keel and T. Tao. " Endpoint Strichartz estimates ". In: *Amer. J. Math.* 120.5 (1998), pp. 955–980. URL: http://muse.jhu.edu/journals/american_journal_of_mathematics/v120/120.5keel.pdf.

References of Chapter 4

[AFW10] D. Arnold, R. S. Falk, and R. Winther. " Finite element exterior calculus: from Hodge theory to numerical stability ". In: *Bull. Amer. Math. Soc.* 47.2 (2010), pp. 281–354.

[AGM06] L. Aceto, P. Ghelardoni, and M. Marletta. " Numerical computation of eigenvalues in spectral gaps of Sturm-Liouville operators ". In: *J. Comput. Appl. Math.* 189.1-2 (2006), pp. 453–470.

[Atk+94] F. V. Atkinson, H. Langer, R. Mennicken, and A. A. Shkalikov. " The essential spectrum of some matrix operators ". In: *Math. Nachr.* 167 (1994), pp. 5–20.

[BB10] L. Boulton and N. Boussaïd. " Non-variational computation of the eigenstates of Dirac operators with radially symmetric potentials " . In: *LMS J. Comput. Math.* 13 (2010), pp. 10–32. DOI: 10.1112/S1461157008000429. URL: http://hal.archives-ouvertes.fr/hal-00308843/PDF/Preprint-DiracNumerical.pdf.

[BBBa] G. R. Barrenechea, L. Boulton, and N. Boussaïd. *Eigenvalue enclosures*. URL: http://hal.archives-ouvertes.fr/hal-00837475.

[BBBb] G. R. Barrenechea, L. Boulton, and N. Boussaïd. *Finite element eigenvalue enclosures for the Maxwell operator*. URL: http://hal.archives-ouvertes.fr/hal-00949589.

[BBBc] G. Barrenechea, L. Boulton, and N. Boussaïd. " Some remarks on the spectral properties of the maxwell operator on rough domains and domains with symmetries ".

[BBB16] G. Barrenechea, L. Boulton, and N. Boussaïd. " Various remarks on the spectral properties of the Maxwell operator on rough domains and domains with symmetries ". 2016.

[BBG00] D. Boffi, F. Brezzi, and L. Gastaldi. " On the problem of spurious eigenvalues in the approximation of linear elliptic problems in mixed form ". In: *Math. Comp.* 69.229 (2000), pp. 121–140.

[BBG98] D. Boffi, F. Brezzi, and L. Gastaldi. "Mixed finite elements for Maxwell's eigenproblem: the question of spurious modes". In: *ENUMATH 97 (Heidelberg)*. 1998, pp. 180–187.

[BBL12] L. Boulton, N. Boussaïd, and M. Lewin. " Generalised Weyl theorems and spectral pollution in the Galerkin method " . In: *J. Spectr. Theory* 2.4 (2012), pp. 329–354. DOI: 10.4171/JST/32. URL: http://hal.archives-ouvertes.fr/hal-00536270/PDF/Weyl32.pdf.

[Beh09] H. Behnke. " Lower and Upper Bounds for Sloshing Frequencies ". In: *Inequalities and Applications* (2009), pp. 13–22.

[Bet+13] T. Betcke, N. J. Higham, V. Mehrmann, C. Schröder, and F. Tisseur. *NLEVP: A Collection of Nonlinear Eigenvalue Problems*. Feb. 2013. DOI: 10.1145/2427023.2427024. URL: http://www.mims.manchester.ac.uk/research/numerical-analysis/nlevp.html.

[BH13a] L. Boulton and A. Hobiny. " On the convergence of the quadratic method ". In: *ArXiv e-prints* (July 2013). arXiv: 1307.0313 [math.NA].

[BH13b] L. Boulton and A. Hobiny. " On the quality of complementary bounds for eigenvalues ". In: *ArXiv e-prints* (Nov. 2013). arXiv: 1311.5181 [math.SP].

[BL07] L. Boulton and M. Levitin. " On Approximation of the Eigenvalues of Perturbed Periodic Schrodinger Operators ". In: *J. Phys. A: Math. Theor.* 40.31 (2007), pp. 9319–9329.

[BM01] H. Behnke and U. Mertins. " Bounds for eigenvalues with the use of finite elements ". In: *Perspectives on Enclosure Methods* (2001), p. 119.

[Bou07] L. Boulton. " Non-variational approximation of discrete eigenvalues of self-adjoint operators ". In: *IMA J. Numer. Anal.* 27.1 (2007), pp. 102–121.

[BS12] L. Boulton and M. Strauss. " Eigenvalue enclosures and convergence for the linearized MHD operator " . In: *BIT* 52.4 (2012), pp. 801–825. DOI: 10.1007/s10543-012-0389-x. URL: http://dx.doi.org/10.1007/s10543-012-0389-x.

[BS90] M. Birman and M. Solomyak. " The self-adjoint Maxwell operator in arbitrary domains ". In: *Leningrad Math. J* 1.1 (1990), pp. 99–115.

[CDL08] É. Cancès, A. Deleurence, and M. Lewin. " Non-perturbative embedding of local defects in crystalline materials " . In: *J. Phys.: Condens. Matter* 20 (2008), p. 294213. DOI: 10.1088/0953-8984/20/29/294213.

[Cha83] F. Chatelin. *Spectral Approximation of Linear Operators*. New York, 1983.

[Dau04] M. Dauge. *Computations for Maxwell equations for the approximation of highly singular solutions*. 2004. URL: http://perso.univ-rennes1.fr/monique.dauge/benchmax.html.

[Dav00] E. B. Davies. " A hierarchical method for obtaining eigenvalue enclosures ". In: *Math. Comp.* 69.232 (2000), pp. 1435–1455.

[Dav98] E. B. Davies. " Spectral enclosures and complex resonances for general self-adjoint operators " . In: *LMS J. Comput. Math.* 1 (1998), pp. 42–74. DOI: 10.1112/S1461157000000140. URL: http://dx.doi.org/10.1112/S1461157000000140.

[DG81] G. W. F. Drake and S. P. Goldman. " Application of discrete-basis-set methods to the Dirac equation " . In: *Phys. Rev. A* 23.5 (May 1981), pp. 2093–2098. DOI: 10.1103/PhysRevA.23.2093.

[DP04] E. B. Davies and M. Plum. " Spectral pollution ". In: *IMA J. Numer. Anal.* 24.3 (2004), pp. 417–438.

[DS02] M. Dauge and M. Suri. " Numerical approximation of the spectra of non-compact operators arising in buckling problems ". In: *J. Numer. Math.* 10.3 (2002), pp. 193–219.

[EG04] A. Ern and J.-L. Guermond. *Theory and practice of finite elements*. Vol. 159. Applied Mathematical Sciences. New York, 2004, pp. xiv+524.

[GA86] F. Goerisch and J. Albrecht. "The convergence of a new method for calculating lower bounds to eigenvalues". In: *Equadiff 6 (Brno, 1985)*. Vol. 1192. Lecture Notes in Math. Berlin, 1986, pp. 303–308.

[Gra82] I. P. Grant. " Conditions for convergence of variational solutions of Dirac's equation in a finite basis " . In: *Phys. Rev. A* 25.2 (Feb. 1982), pp. 1230–1232. DOI: 10.1103/PhysRevA.25.1230.

[KLT04] M. Kraus, M. Langer, and C. Tretter. " Variational principles and eigenvalue estimates for unbounded block operator matrices and applications ". In: *J. Comput. Appl. Math.* 171.1-2 (2004), pp. 311–334.

[Kut84] W. Kutzelnigg. " Basis set expansion of the Dirac operator without variational collapse ". In: *Int. J. Quantum Chemistry* 25 (1984), pp. 107–129.

[LS04] M. Levitin and E. Shargorodsky. " Spectral pollution and second-order relative spectra for self-adjoint operators ". In: *IMA J. Numer. Anal.* 24.3 (2004), pp. 393–416.

[LS10] M. Lewin and É. Séré. " Spectral pollution and how to avoid it (with applications to Dirac and periodic Schrödinger operators) " . In: *Proc. Lond. Math. Soc. (3)* 100.3 (2010), pp. 864–900. DOI: 10.1112/plms/pdp046. URL: http://dx.doi.org/10.1112/plms/pdp046.

[Mar10] M. Marletta. " Neumann-Dirichlet maps and analysis of spectral pollution for non-self-adjoint elliptic PDEs with real essential spectrum ". In: *IMA J. Numer. Anal.* 30.4 (2010), pp. 887–897.

[Mon03] P. Monk. *Finite element methods for Maxwell's equations*. Cambridge, 2003.

[Rap+97] J. Rappaz, J. Sanchez Hubert, E. Sanchez Palencia, and D. Vassiliev. " On spectral pollution in the finite element approximation of thin elastic "membrane" shells ". In: *Numer. Math.* 75.4 (1997), pp. 473–500.

[SH84] R. E. Stanton and S. Havriliak. " Kinetic balance: A partial solution to the problem of variational safety in Dirac calculations " . In: *J. Chem. Phys.* 81.4 (1984), pp. 1910–1918. DOI: 10.1063/1.447865. URL: http://link.aip.org/link/?JCP/81/1910/1.

[SW93] G. Stolz and J. Weidmann. " Approximation of isolated eigenvalues of ordinary differential operators ". In: *J. Reine Angew. Math.* 445 (1993), pp. 31–44.

[SW95] G. Stolz and J. Weidmann. " Approximation of isolated eigenvalues of general singular ordinary differential operators ". In: *Results Math.* 28.3-4 (1995), pp. 345–358.

[Wei74] H. F. Weinberger. *Variational methods for eigenvalue approximation*. Based on a series of lectures presented at the NSF-CBMS Regional Conference on Approximation of Eigenvalues of Differential Operators, Vanderbilt University, Nashville, Tenn., June 26–30, 1972, Conference Board of the Mathematical Sciences Regional Conference Series in Applied Mathematics, No. 15. 1974, pp. v+160.

[ZM95] S. Zimmermann and U. Mertins. " Variational bounds to eigenvalues of self-adjoint eigenvalue problems with arbitrary spectrum ". In: *Z. Anal. Anwendungen* 14.2 (1995), pp. 327–345.

References of Chapter 5

[ABG96] W. O. Amrein, A. Boutet de Monvel, and V. Georgescu. *C_0-groups, commutator methods and spectral theory of N-body Hamiltonians*. Vol. 135. Progress in Mathematics. Basel, 1996, pp. xiv+460.

[Ast+06] M. Astaburuaga, O. Bourget, V. Cortés, and C. Fernández. " Floquet operators without singular continuous spectrum. " In: *J. Funct. Anal.* 238.2 (2006), pp. 489–517. DOI: 10.1016/j.jfa.2006.03.028.

[BDF11] N. Boussaïd, P. D'Ancona, and L. Fanelli. " Virial identity and weak dispersion for the magnetic Dirac equation " . In: *J. Math. Pures Appl. (9)* 95.2 (2011), pp. 137–150. DOI: 10.1016/j.matpur.2010.10.004. URL: http://hal.archives-ouvertes.fr/hal-00430346/PDF/diracsmoo-20091218.pdf.

[BG10] N. Boussaïd and S. Golénia. " Limiting absorption principle for some long range perturbations of Dirac systems at threshold energies " . In: *Comm. Math. Phys.* 299.3 (2010), pp. 677–708. DOI: 10.1007/s00220-010-1099-3. URL: http://hal.archives-ouvertes.fr/hal-00392422/PDF/LAPDLRvHAL20090608.pdf.

[BH10] J.-F. Bony and D. Häfner. " Low frequency resolvent estimates for long range perturbations of the Euclidean Laplacian " . In: *Math. Res. Lett.* 17.2 (2010), pp. 303–308. DOI: 10.4310/MRL.2010.v17.n2.a9. URL: http://dx.doi.org/10.4310/MRL.2010.v17.n2.a9.

[BKM96] A. Boutet de Monvel, G. Kazantseva, and M. Mantoiu. " Some anisotropic Schrödinger operators without singular spectrum ". In: *Helv. Phys. Acta* 69.1 (1996), pp. 13–25.

[BM97] A. Boutet de Monvel and M. Măntoiu. *The method of the weakly conjugate operator.* Apagyi, Barnabás (ed.) et al., Inverse and algebraic quantum scattering theory. Proceedings of a conference, held at Lake Balaton, Hungary. 3–7 September 1996. Berlin: Springer. Lect. Notes Phys. 488, 204-226 (1997). 1997.

[Bou11] J.-M. Bouclet. " Low frequency estimates for long range perturbations in divergence form " . In: *Canad. J. Math.* 63.5 (2011), pp. 961–991. DOI: 10.4153/CJM-2011-022-9. URL: http://dx.doi.org/10.4153/CJM-2011-022-9.

[Bur+04] N. Burq, F. Planchon, J. G. Stalker, and A. S. Tahvildar-Zadeh. " Strichartz estimates for the wave and Schrödinger equations with potentials of critical decay " . In: *Indiana Univ. Math. J.* 53.6 (2004), pp. 1665–1680. DOI: 10.1512/iumj.2004.53.2541. URL: http://dx.doi.org/10.1512/iumj.2004.53.2541.

[CS88] P. Constantin and J.-C. Saut. " Local smoothing properties of dispersive equations " . In: *J. Amer. Math. Soc.* 1.2 (1988), pp. 413–439. DOI: 10.2307/1990923. URL: http://dx.doi.org/10.2307/1990923.

[DES00] J. Dolbeault, M. J. Esteban, and E. Séré. " On the eigenvalues of operators with gaps. Application to Dirac operators " . In: *J. Funct. Anal.* 174.1 (2000), pp. 208–226. DOI: 10.1006/jfan.1999.3542. URL: http://dx.doi.org/10.1006/jfan.1999.3542.

[DS09a] J. Dereziński and E. Skibsted. " Quantum scattering at low energies " . In: *J. Funct. Anal.* 257.6 (2009), pp. 1828–1920. DOI: 10.1016/j.jfa.2009.05.026. URL: http://dx.doi.org/10.1016/j.jfa.2009.05.026.

[DS09b] J. Dereziński and E. Skibsted. " Scattering at zero energy for attractive homogeneous potentials " . In: *Ann. Henri Poincaré* 10.3 (2009), pp. 549–571. DOI: 10.1007/s00023-009-0408-x. URL: http://dx.doi.org/10.1007/s00023-009-0408-x.

[FGS08] J. Fröhlich, M. Griesemer, and I. M. Sigal. “ Spectral theory for the standard model of non-relativistic QED ” . In: *Comm. Math. Phys.* 283.3 (2008), pp. 613–646. DOI: 10.1007/s00220-008-0506-5. URL: http://dx.doi.org/10.1007/s00220-008-0506-5.

[FGS11] J. Fröhlich, M. Griesemer, and I. M. Sigal. “ Spectral renormalization group and local decay in the standard model of non-relativistic quantum electrodynamics ” . In: *Rev. Math. Phys.* 23.2 (2011), pp. 179–209. DOI: 10.1142/S0129055X11004266. URL: http://dx.doi.org/10.1142/S0129055X11004266.

[FL74] W. G. Faris and R. B. Lavine. “ Commutators and self-adjointness of Hamiltonian operators ”. In: *Comm. Math. Phys.* 35 (1974), pp. 39–48.

[FS04] S. Fournais and E. Skibsted. “ Zero energy asymptotics of the resolvent for a class of slowly decaying potentials ”. In: *Math. Z.* 248.3 (2004), pp. 593–633.

[GH08] C. Guillarmou and A. Hassell. “ Resolvent at low energy and Riesz transform for Schrödinger operators on asymptotically conic manifolds. I ” . In: *Math. Ann.* 341.4 (2008), pp. 859–896. DOI: 10.1007/s00208-008-0216-5. URL: http://dx.doi.org/10.1007/s00208-008-0216-5.

[GH09] C. Guillarmou and A. Hassell. “ Resolvent at low energy and Riesz transform for Schrödinger operators on asymptotically conic manifolds. II ”. In: *Ann. Inst. Fourier (Grenoble)* 59.4 (2009), pp. 1553–1610. URL: http://aif.cedram.org/item?id=AIF_2009__59_4_1553_0.

[GM01] V. Georgescu and M. Măntoiu. “ On the spectral theory of singular Dirac type Hamiltonians ”. In: *J. Operator Theory* 46.2 (2001), pp. 289–321.

[IM99] A. Iftimovici and M. Măntoiu. “ Limiting absorption principle at critical values for the Dirac operator ”. In: *Lett. Math. Phys.* 49.3 (1999), pp. 235–243.

[Jac75] J. D. Jackson. *Classical electrodynamics*. Second. 1975, pp. xxii+848.

[JK79] A. Jensen and T. Kato. “ Spectral properties of Schrödinger operators and time-decay of the wave functions ”. In: *Duke Math. J.* 46.3 (1979), pp. 583–611.

[JN01] A. Jensen and G. Nenciu. “ A unified approach to resolvent expansions at thresholds ”. In: *Rev. Math. Phys.* 13.6 (2001), pp. 717–754.

[Lav71] R. B. Lavine. “ Commutators and scattering theory. I. Repulsive interactions ”. In: *Comm. Math. Phys.* 20 (1971), pp. 301–323.

[Mor68] C. S. Morawetz. “ Time decay for the nonlinear Klein-Gordon equations ”. In: *Proc. Roy. Soc. Ser. A* 306 (1968), pp. 291–296.

[Nak94] S. Nakamura. “ Low energy asymptotics for Schrödinger operators with slowly decreasing potentials ”. In: *Comm. Math. Phys.* 161.1 (1994), pp. 63–76. URL: http://projecteuclid.org/euclid.cmp/1104269792.

[Put67] C. R. Putnam. *Commutation properties of Hilbert space operators and related topics*. Ergebnisse der Mathematik und ihrer Grenzgebiete, Band 36. 1967, pp. xi+167.

[PV08] B. Perthame and L. Vega. “ Energy concentration and Sommerfeld condition for Helmholtz equation with variable index at infinity ” . In: *Geom. Funct. Anal.* 17.5 (2008), pp. 1685–1707. DOI: 10.1007/s00039-007-0635-6. URL: http://dx.doi.org/10.1007/s00039-007-0635-6.

[PV99] B. Perthame and L. Vega. " Morrey-Campanato estimates for Helmholtz equations " . In: *J. Funct. Anal.* 164.2 (1999), pp. 340–355. DOI: 10.1006/jfan.1999.3391. URL: http://dx.doi.org/10.1006/jfan.1999.3391.

[Ric06] S. Richard. " Some improvements in the method of the weakly conjugate operator ". In: *Lett. Math. Phys.* 76.1 (2006), pp. 27–36.

[Roy] J. Royer. " Limiting absorption principle for the dissipative Helmholtz equation ". URL: http://hal.archives-ouvertes.fr/hal-00380641/en/.

[RS04] I. Rodnianski and W. Schlag. " Time decay for solutions of Schrödinger equations with rough and time-dependent potentials " . In: *Invent. Math.* 155.3 (2004), pp. 451–513. DOI: 10.1007/s00222-003-0325-4. URL: http://dx.doi.org/10.1007/s00222-003-0325-4.

[RS78] M. Reed and B. Simon. *Methods of modern mathematical physics. IV. Analysis of operators*. New York, 1978, pp. xv+396.

[Sjö87] P. Sjölin. " Regularity of solutions to the Schrödinger equation " . In: *Duke Math. J.* 55.3 (1987), pp. 699–715. DOI: 10.1215/S0012-7094-87-05535-9. URL: http://dx.doi.org/10.1215/S0012-7094-87-05535-9.

[Tha92] B. Thaller. *The Dirac equation*. Texts and Monographs in Physics. Berlin, 1992, pp. xviii+357. DOI: 10.1007/978-3-662-02753-0. URL: http://dx.doi.org/10.1007/978-3-662-02753-0.

[Veg88] L. Vega. " Schrödinger equations: pointwise convergence to the initial data " . In: *Proc. Amer. Math. Soc.* 102.4 (1988), pp. 874–878. DOI: 10.2307/2047326. URL: http://dx.doi.org/10.2307/2047326.

[VW10] A. Vasy and J. Wunsch. " Positive commutators at the bottom of the spectrum " . In: *J. Funct. Anal.* 259.2 (2010), pp. 503–523. DOI: 10.1016/j.jfa.2010.04.012. URL: http://dx.doi.org/10.1016/j.jfa.2010.04.012.

[Yaf82] D. R. Yafaev. " The low energy scattering for slowly decreasing potentials ". In: *Comm. Math. Phys.* 85.2 (1982), pp. 177–196. URL: http://projecteuclid.org/euclid.cmp/1103921410.

References of Chapter 6

[AG74] W. O. Amrein and V. Georgescu. " On the characterization of bound states and scattering states in quantum mechanics ". In: *Helv. Phys. Acta* 46 (1973/74), pp. 635–658.

[BCC12a] N. Boussaïd, M. Caponigro, and T. Chambrion. " Approximate controllability of the Schrödinger equation with a polarizability term " . In: *Decision and Control (CDC), 2012 IEEE 51st Annual Conference on*. IEEE. 2012, pp. 3024–3029. DOI: 10.1109/CDC.2012.6426619. URL: http://hal.archives-ouvertes.fr/hal-00784881/PDF/Quadratique13.pdf.

[BCC12b] N. Boussaïd, M. Caponigro, and T. Chambrion. " Implementation of logical gates on infinite dimensional quantum oscillators ". In: *American Control Conference (ACC), 2012*. IEEE. 2012, pp. 5825–5830. URL: http://hal.archives-ouvertes.fr/hal-00637115/PDF/QG%5C_ACC%5C_0.6.pdf.

[BCC12c] N. Boussaïd, M. Caponigro, and T. Chambrion. " Periodic control laws for bilinear quantum systems with discrete spectrum ". In: *American Control Conference (ACC), 2012*. IEEE. 2012, pp. 5819–5824. URL: http://hal.archives-ouvertes.fr/hal-00637116/PDF/FEPS%5C_ACC%5C_3.pdf.

[BCC12d] N. Boussaïd, M. Caponigro, and T. Chambrion. " Small time reachable set of bilinear quantum systems " . In: *Decision and Control (CDC), 2012 IEEE 51st Annual Conference on*. IEEE. 2012, pp. 1083–1087. DOI: 10.1109/CDC.2012.6426208. URL: http://hal.archives-ouvertes.fr/hal-00710040/PDF/Time06.pdf.

[BCC12e] N. Boussaïd, M. Caponigro, and T. Chambrion. " Which notion of energy for bilinear quantum systems? " In: *proceeding of the 4th IFAC Workshop on Lagrangian and Hamiltonian Methods for Non Linear Control, pp 226-230, 29-31 août 2012*. 2012, pp. 226–230. DOI: 10.3182/20120829-3-IT-4022.00034. URL: http://hal.archives-ouvertes.fr/hal-00784890/PDF/Energy4.pdf.

[BCC13a] N. Boussaïd, M. Caponigro, and T. Chambrion. " Energy Estimates for Low Regularity Bilinear Schrödinger Equations " . In: *Control of Systems Governed by Partial Differential Equations*. Vol. 1. 1. 2013, pp. 25–30. DOI: 10.3182/20130925-3-FR-4043.00046. URL: http://hal.archives-ouvertes.fr/hal-00784876/PDF/cpde09.pdf.

[BCC13b] N. Boussaïd, M. Caponigro, and T. Chambrion. " Total variation of the control and energy of bilinear quantum systems " . In: *Decision and Control (CDC), 2013 IEEE 52nd Annual Conference on*. Dec. 2013, pp. 3714–3719. DOI: 10.1109/CDC.2013.6760455. URL: http://hal.archives-ouvertes.fr/hal-00800548/PDF/BVefficiency09.pdf.

[BCC13c] N. Boussaïd, M. Caponigro, and T. Chambrion. " Weakly coupled systems in quantum control " . In: *IEEE Trans. Automat. Control* 58.9 (2013), pp. 2205–2216. DOI: 10.1109/TAC.2013.2255948.

[BCC14a] N. Boussaïd, M. Caponigro, and T. Chambrion. *Approximate controllability of the Schrödinger Equation with a polarizability term in higher Sobolev norms*. June 2014. URL: http://hal.archives-ouvertes.fr/hal-01006178.

[BCC14b] N. Boussaïd, M. Caponigro, and T. Chambrion. *Efficient finite dimensional approximations for the bilinear Schrodinger equation with bounded variation controls*. 2014. URL: http://hal.archives-ouvertes.fr/hal-01003056.

[BCC14c] N. Boussaïd, M. Caponigro, and T. Chambrion. *Regular propagators of bilinear quantum systems*. June 2014. URL: http://hal.archives-ouvertes.fr/hal-01016299.

[BCT14] K. Beauchard, J.-M. Coron, and H. Teismann. " Minimal time for the bilinear control of Schr\"odinger equations ". In: *ArXiv e-prints* (Jan. 2014). arXiv: 1401.6828 [math.AP].

[Bea05] K. Beauchard. " Local controllability of a 1-D Schrödinger equation ". In: *J. Math. Pures Appl.* 84.7 (2005), pp. 851–956.

[BL10] K. Beauchard and C. Laurent. " Local controllability of 1D linear and nonlinear Schrödinger equations with bilinear control ". In: *J. Math. Pures Appl.* 94.5 (2010), pp. 520–554.

[BMS82] J. M. Ball, J. E. Marsden, and M. Slemrod. " Controllability for distributed bilinear systems ". In: *SIAM J. Control Optim.* 20.4 (1982), pp. 575–597.

[Bos+12] U. Boscain, M. Caponigro, T. Chambrion, and M. Sigalotti. “ A weak spectral condition for the controllability of the bilinear Schrödinger equation with application to the control of a rotating planar molecule ”. In: *Comm. Math. Phys.* 311.2 (2012), pp. 423–455.

[Cha+09] T. Chambrion, P. Mason, M. Sigalotti, and U. Boscain. “ Controllability of the discrete-spectrum Schrödinger equation driven by an external field ”. In: *Ann. Inst. H. Poincaré Anal. Non Linéaire* 26.1 (2009), pp. 329–349.

[Cha12] T. Chambrion. “ Periodic excitations of bilinear quantum systems ” . In: *Automatica J. IFAC* 48.9 (2012), pp. 2040–2046. DOI: 10.1016/j.automatica.2012.03.031. URL: http://dx.doi.org/10.1016/j.automatica.2012.03.031.

[Ens78] V. Enss. “ Asymptotic completeness for quantum mechanical potential scattering. I. Short range potentials ”. In: *Comm. Math. Phys.* 61.3 (1978), pp. 285–291.

[Kat53] T. Kato. “ Integration of the equation of evolution in a Banach space ”. In: *J. Math. Soc. Japan* 5 (1953), pp. 208–234.

[Kat70] T. Kato. “ Linear evolution equations of “hyperbolic” type ”. In: *J. Fac. Sci. Univ. Tokyo Sect. I* 17 (1970), pp. 241–258.

[MR04] M. Mirrahimi and P. Rouchon. “ Controllability of quantum harmonic oscillators ” . In: *IEEE Trans. Automat. Control* 49.5 (2004), pp. 745–747. DOI: 10.1109/TAC.2004.825966. URL: http://dx.doi.org/10.1109/TAC.2004.825966.

[Nat55] I. P. Natanson. *Theory of functions of a real variable.* Translated by Leo F. Boron with the collaboration of Edwin Hewitt. 1955, p. 277.

[Ner09] V. Nersesyan. “ Growth of Sobolev norms and controllability of the Schrödinger equation ”. In: *Comm. Math. Phys.* 290.1 (2009), pp. 371–387.

[Rue69] D. Ruelle. “ A remark on bound states in potential-scattering theory ”. In: *Nuovo Cimento A (10)* 61 (1969), pp. 655–662.

[Tur00] G. Turinici. “ On the controllability of bilinear quantum systems ”. In: *Mathematical models and methods for ab initio Quantum Chemistry*. Ed. by M. Defranceschi and C. Le Bris. Vol. 74. Lecture Notes in Chemistry. 2000.

References of Chapter 7

[BC] N. Boussaïd and A. Comech. “ Linear stability of the nonlinear Dirac equation in the nonrelativistic limit ”.

[BC12a] G. Berkolaiko and A. Comech. “ On spectral stability of solitary waves of nonlinear Dirac equation in 1D ” . In: *Math. Model. Nat. Phenom.* 7.2 (2012), pp. 13–31. DOI: 10.1051/mmnp/20127202. URL: http://dx.doi.org/10.1051/mmnp/20127202.

[BC12b] N. Boussaïd and A. Comech. *On spectral stability of the nonlinear Dirac equation.* 2012. arXiv: 1211.3336 [math.AP].

[BC12c] N. Boussaïd and S. Cuccagna. “ On stability of standing waves of nonlinear Dirac equations ” . In: *Comm. Partial Differential Equations* 37.6 (2012), pp. 1001–1056. DOI: 10.1080/03605302.2012.665973. URL: http://hal.archives-ouvertes.fr/hal-00578790/PDF/StabDirac20120103.pdf.

[BG87] A. Berthier and V. Georgescu. " On the point spectrum of Dirac operators " . In: *J. Funct. Anal.* 71.2 (1987), pp. 309–338. DOI: 10.1016/0022-1236(87)90007-3. URL: http://dx.doi.org/10.1016/0022-1236(87)90007-3.

[BL83] H. Berestycki and P.-L. Lions. " Nonlinear scalar field equations. I. Existence of a ground state " . In: *Arch. Rational Mech. Anal.* 82.4 (1983), pp. 313–345. DOI: 10.1007/BF00250555. URL: http://dx.doi.org/10.1007/BF00250555.

[Bou06] N. Boussaïd. " Stable directions for small nonlinear Dirac standing waves " . In: *Comm. Math. Phys.* 268.3 (2006), pp. 757–817. DOI: 10.1007/s00220-006-0112-3. URL: http://hal.archives-ouvertes.fr/hal-00016041/PDF/Article-StabilizationSmallDirac%20SolitonNonResonantCaseFinal.pdf.

[Bou08] N. Boussaïd. " On the asymptotic stability of small nonlinear Dirac standing waves in a resonant case " . In: *SIAM J. Math. Anal.* 40.4 (2008), pp. 1621–1670. DOI: 10.1137/070684641. URL: http://hal.archives-ouvertes.fr/hal-00116269/PDF/Article-2-StabilizationSmallDir%20acSolitonResonantCaseFinal41.pdf.

[CGG14] A. Comech, M. Guan, and S. Gustafson. " On linear instability of solitary waves for the nonlinear Dirac equation " . In: *Ann. Inst. H. Poincaré Anal. Non Linéaire* 31.3 (2014), pp. 639–654. DOI: 10.1016/j.anihpc.2013.06.001. URL: http://dx.doi.org/10.1016/j.anihpc.2013.06.001.

[Cha+08] S.-M. Chang, S. Gustafson, K. Nakanishi, and T.-P. Tsai. " Spectra of linearized operators for NLS solitary waves " . In: *SIAM J. Math. Anal.* 39.4 (2007/08), pp. 1070–1111. DOI: 10.1137/050648389. URL: http://dx.doi.org/10.1137/050648389.

[CHS12] O. Costin, M. Huang, and W. Schlag. " On the spectral properties of $L_\pm$ in three dimensions " . In: *Nonlinearity* 25 (Jan. 2012), pp. 125–164. DOI: 10.1088/0951-7715/25/1/125. arXiv: 1107.0323 [math.AP].

[CL82] T. Cazenave and P.-L. Lions. " Orbital stability of standing waves for some nonlinear Schrödinger equations ". In: *Comm. Math. Phys.* 85.4 (1982), pp. 549–561. URL: http://projecteuclid.org/euclid.cmp/1103921547.

[CV86] T. Cazenave and L. Vázquez. " Existence of localized solutions for a classical nonlinear Dirac field ". In: *Comm. Math. Phys.* 105.1 (1986), pp. 35–47. URL: http://projecteuclid.org/euclid.cmp/1104115255.

[GSS87] M. Grillakis, J. Shatah, and W. Strauss. " Stability theory of solitary waves in the presence of symmetry. I " . In: *J. Funct. Anal.* 74.1 (1987), pp. 160–197. DOI: 10.1016/0022-1236(87)90044-9. URL: http://dx.doi.org/10.1016/0022-1236(87)90044-9.

[Gua08] M. Guan. " Solitary Wave Solutions for the Nonlinear Dirac Equations ". In: *ArXiv e-prints* (Dec. 2008). arXiv: 0812.2273 [math.AP].

[SS85] J. Shatah and W. Strauss. " Instability of nonlinear bound states ". In: *Comm. Math. Phys.* 100.2 (1985), pp. 173–190.

[Tha92] B. Thaller. *The Dirac equation*. Texts and Monographs in Physics. Berlin, 1992, pp. xviii+357. DOI: 10.1007/978-3-662-02753-0. URL: http://dx.doi.org/10.1007/978-3-662-02753-0.

[VK73] N. G. Vakhitov and A. A. Kolokolov. " Stationary solutions of the wave equation in the medium with nonlinearity saturation " . In: *Radiophys. Quantum Electron.* 16 (1973), pp. 783–789. DOI: 10.1007/BF01031343.

[Wei85] M. I. Weinstein. “ Modulational stability of ground states of nonlinear Schrödinger equations ”. In: *SIAM J. Math. Anal.* 16.3 (1985), pp. 472–491.

[Wei86] M. I. Weinstein. “ Lyapunov stability of ground states of nonlinear dispersive evolution equations ”. In: *Comm. Pure Appl. Math.* 39.1 (1986), pp. 51–67.

Illustration of OLEA europaea L. 109 (Olea europaea L., olive)
Köhler's Medizinal-Pflanzen in naturgetreuen Abbildungen mit kurz erläuterndem

Atlas zur Pharmacopoea germanica, Volume 2 of 3.

Ce mémoire est consacré à l'étude de quelques problèmes issus de la mécanique quantique relativiste et non relativiste.

Dans une première partie, je décris mes travaux sur l'analyse de la pollution spectrale. Je présente dans un premier temps les résultats de stabilité par perturbation de ce phénomène de la théorie spectrale numérique. Puis je détaille l'analyse de deux méthodes d'approximation du spectre exemptes de pollution : la méthode du second ordre appliquée à des opérateurs de Dirac et la méthode de Davies et Plum appliquée, entre autres, à l'opérateur de Maxwell dans une cavité bornée.

Dans une seconde partie, je présente deux analyses des propriétés dispersives de l'opérateur de Dirac. La première porte sur les estimations de Kato pour des perturbations coulombiennes obtenues par des méthodes de Mourre. La seconde s'intéresse à des estimations de Morawetz pour des perturbations magnétiques.

La troisième partie décrit l'ensemble des résultats obtenus en théorie du contrôle bilinéaire d'équations de Schrödinger. Il s'agit essentiellement de résultats de contrôlabilité approchée avec régularité faible en temps ou de résultats de non contrôlabilité. Des résultats quantitatifs sur le temps ou l'énergie de contrôle sont également présentés.

La dernière partie décrit l'analyse de la stabilité de solutions stationnaires d'équations de Dirac non linéaires. Une analyse des propriétés spectrales de la linéarisation donne des résultats de stabilité linéaire alors que l'analyse des résonances non linéaires permet de préciser les propriétés de stabilité asymptotique.
Mots clés : mécanique quantique, mécanique quantique relativiste, pollution spectrale, opérateur de Dirac, opérateur de Maxwell, estimations de Kato, estimations de Mourre, estimations de Morawetz, estimations de Strichartz, contrôle bilinéaire, contrôlabilité approchée, stabilité linéaire, stabilité asymptotique.

Non linear models from relativistic quantum mechanics : spectral and asymptotic analysis and related problems.

This thesis is devoted to some problems from relativistic and non relativistic mechanics.

In a first part, I describe my work on spectral pollution. I present first the results on the stability by perturbation of this phenomenon from numerical spectral theory. Then I detail the analysis of two methods of approximation of the spectrum free from any pollution : the quadratic projective method applied to Dirac operators and the Davies-Plum method applied, among others, to the Maxwell operator in a bounded cavity.

In a second part, I present two analysis on the dispersive properties of the Dirac operator. The first one is on Kato smoothness estimates for coulombic type perturbations obtained by Mourre's methods. The second one is on Morawetz estimates for magnetic perturbations.

The third part describes the results on the bilinear control of Schrödinger equations. It is essentially results on approximate controllability with low time regularity and non controllability. Some quantitative results on the time and energy control are also presented.

The last part describes the analysis of the stability of stationary solutions of non linear Dirac equations. An analysis of the spectral properties of the linearisation gives results on the linear stability while the analysis of non linear resonances gives asymptotic stability properties.
Keywords: quantum mechanics, relativistic quantum mechanics, spectral pollution, Dirac operators, Maxwell operator, Kato smoothness estimates, Mourre estimates, Morawetz estimates, Strichartz estimates, bilinear control, approximate controllability, linear stability, asymptotic stability.

Laboratoire de Mathématiques de Besançon, Université de Franche-Comté, CNRS UMR 6623, 16, route de Gray, 25030 Besançon, France.