The Dirac equation in solid state physics and non-linear optics

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Résumé

L'équation de Dirac non linéaire en physique du solide et en optique non linéaire.

Cette thèse porte sur l'étude de certains modèles issus de la physique du solide et de l'optique non linéaire qui font intervenir l'opérateur de Dirac. Ces dernières années, de nouveaux matériaux bidimensionnels aux propriétés surprenantes ont été découverts, le plus connu étant le graphène. Dans ces matériaux, les électrons du niveau de Fermi ont une masse apparente nulle, et peuvent être décrits par l'équation de Dirac sans masse. Un tel phénomène apparaît dans des situations très générales, pour les matériaux bidimensionnels ayant une structure périodique en "nid d'abeille". La présence d'une perturbation extérieure, sous certaines hypothèses, correspond à un terme de masse dans l'équation de Dirac efficace. De plus, la prise en compte d'interactions mène à des équations non linéaires, qui apparaissent également dans l'étude des paquets d'ondes lumineuses dans certaines fibres optiques. Récemment, des équation de Dirac non linéaires sur des graphes quantiques on été proposées comme modèles efficaces pour des guides d'ondes.

Le but de cette thèse est d'étudier l'existence et la multiplicité de solutions stationnaires de ces équations avec termes non linéaires sous-critiques et critiques. Du point de vue mathématique, on doit résoudre les équations d'Euler-Lagrange de fonctionnelles d'énergie fortement indéfinies faisant intervenir l'opérateur de Dirac. Il s'agit en particulier d'étudier le cas des non-linéarités avec exposant critique, encore mal comprises pour ce type de fonctionnelle, et qui apparaissent naturellement en optique non linéaire.

Le premier chapitre est consacré à une discussion des motivations physiques de cette thèse et notamment des modèles physiques où l'équation de Dirac intervient comme équation efficace. Ensuite, les propriétés spectrales de l'opérateur de Dirac en dimension deux et dans le cas de certains graphes quantiques sont présentées dans le deuxième chapitre. Des résultats d'éxistence et de localisation pour des équations de Dirac non linéaires font l'objet du troisième chapitre. En particulier, nous démontrons l'existence de solutions stationnaires pour des équations de Dirac cubique en dimension deux, qui

sont critiques pour les injections de Sobolev. Le quatrième chapitre porte sur l'étude d'un modèle pour la conduction d'électrons dans des échantillons de graphène. Il s'agit d'étudier une équation de type Dirac-Hartree, pour laquelle nous démontrons l'existence d'une infinité de solutions stationnaires. Finalement, le dernier chapitre est consacré à l'étude d'une famille déquations de Dirac non linéaires sur des graphes quantiques. Nous prouvons l'existence et la multiplicité de solutions, dont nous étudions la limite non relativiste. Plus précisement, dans certains régimes de paramètres, les solutions de l'équation de Dirac non linéaires convergent vers celles de l'équation de Schrödinger avec le même type de non-linéarité.

The nonlinear Dirac equation in solid state physics and nonlinear optics.

The present thesis deals with nonlinear Dirac equations arising in solid state physics and nonlinear optics. Recently new two dimensional material possessing surprising properties have been discovered, the most famous being graphene. In this materials, electrons at the Fermi level can be described by a massless Dirac equations.This holds, more generally, for two dimensional honeycomb structures, under fairly general hypothesis. The effect of a suitable external perturbations can be described adding a mass term in the effective Dirac operator. Moreover, taking into account interactions naturally leads to nonlinear Dirac equations, which also appear in the description of the propagation of light pulses in optical fibers. Nonlinear Dirac equations have also been recently proposed as effective models for waveguides arrays.

The aim of this thesis is to investigate existence and multiplicity properties of stationary solutions to sub-critical and critical Dirac equations, which arise as Euler-Lagrange equations of strongly indefinite functionals involving the Dirac operator. We have to deal with the case of critical nonlinearities, still poorly understood (at least in the low dimensional case), and which appear naturally in nonlinear optics.

The first chapter is devoted to the physical motivations of our work, and more precisely to the presentation of the physical models where the Dirac equation appears as effective model. The spectral properties of the Dirac operator in dimension two and for the case of metric graphs with particular vertex conditions are presented in the second chapter. Existence and localization results for nonlinear Dirac equations in two dimensions are the object of the third chapter. More precisely, we prove the existence of stationary solutions for cubic two dimensional Dirac equations, which are critical for the Sobolev embedding. The fourth chapter deals with a model for electron conductions in graphene samples. We study a Dirac-Hartree equation for which we prove the existence of infinitely many solutions. Finally, in the last chapter we study a class of nonlinear Dirac equations on quantum graphs. We prove the existence of multiple solutions and study the non relativistic limit. More precisely, we show that for a certain choice of parameters the solutions of nonlinear Dirac equations converge toward the solutions of the Schrödinger equation with the same type of nonlinearity.

Contents

Chapter 1

Nouveaux matériaux, graphes quantiques et l'équation de Dirac

L'équation de Dirac a été largement utilisée dans le cadre de la physique quantique relativiste [52] pour décrire des particules elémentaires (électrons, quarks, neutrinos...). Ces dernières années des nouveaux matériaux , appelés *Dirac materials*, ont été découverts. Leur particularité est que les électrons au niveau de Fermi peuvent être décrits par une équation de Dirac sans masse. Dans ces matériaux les bandes de valence et de conduction ont un croisement conique au niveau de Fermi, d'où l'apparition de l'opérateur de Dirac comme opérateur effectif décrivant le comportement des électrons. Ce type de phénomène apparaît de façon générale dans des structures périodiques hexagonales en 2D, et qui peuvent donc être considerées comme des semiconducteurs *à gap nul*, et dans l'étude des états de surface pour certains *isolants topologiques* (voir [39]). La propriété de faire apparaître des fermions de masse nulle décrits par une équation relativiste est particuliérement intéressante pour la physique fondamentale. Plus précisément, dans ces systemes la vitesse de la lumière c est remplacée par la vitesse de Fermi $v_F \simeq c/300$. Cela pourrait permettre, en principe, de tester des éffets relativistes dans des systèmes de physique du solide et donc à des échelles d'énergie facilement accesibles et contrôlables [75].

Dans la suite de ce chapitre nous allons nous concentrer sur le cas particulier du graphène, le plus fameux de ces nouveaux matériaux. Nous montrerons comment les cones de Dirac apparaissent dans la déscription du graphène dans le cadre d'un modèle de *tight-binding.* Ensuite, nous allons illustrer des résultats récents dus à Fefferman and Weinstein [56, 57] qui prouvent rigoureusement l'éxistence de croisements coniques pour les bandes de dispersion pour opérateurs de Schrödinger périodiques ayant les symétries d'un réseau hexagonal, sous des hypothèses très générales. Ils montrent aussi un resultat de validité de Dirac comme équation effective pour la description de la dynamique linéaire pour l'équation de Schrödinger correspondante, pour des paquets d'ondes concentrés (en fréquence) autour des croisement coniques des bandes. Le cas non linéaire sera traité dans les chapitres suivants. Le reste de ce chapitre est consacré à l'étude de certaines modèles qui permettent de décrire des échantillons de graphène de tailles finie et à un bref rappel sur les graphes quantiques, qui sera utile dans la suite de la thèse.

1.1 Un exemple célèbre: le graphène

Le graphène est un matériau bidimensionnel cristallin d'un seul atome d'épaisseur. Il est constitué par un réseau hexagonal d'atomes de carbone, et il est l'élément structurel de base d'autres formes allotropiques du carbone, comme les nanotubes, le graphite ou le fullerènes (voir e.g. [39, 79]). Son existence a été théorisée par Wallace dans les années '40 [123]. Il a été fabriqué pour la première fois en 2004 par A. Geim and K. Novoselov, qui ont reçu le prix Nobel en 2010 pour cette découverte surprenante.

La structure du graphène correspond à un réseau hexagonal $\mathbb{H}$, donné par la superposition de deux réseaux triangulaires $\mathbb{H} = (A + \Lambda) \cup (B + \Lambda)$ (voir Fig. 1.1), où

$$\Lambda = \mathbb{Z}a_1 \oplus \mathbb{Z}a_2$$

et les vecteurs $a_1, a_2 \in \mathbb{R}^2$ sont linéairement indépendants. Le réseau dual

$$\mathbb{H}^* = \left\{ k \in \mathbb{R}^2 : k \cdot a \in 2\pi\mathbb{Z}, \forall a \in \Lambda \right\}$$

est encore hexagonal et sa cellule élementaire $\mathcal{B}$ est appelé *zone de Brillouin* du réseau. Supposons que Λ soit un réseau avec un nombre fini de sommets $N = |\mathbb{H}|$. En l'absence de potentiels extérieurs et de déformations du réseau le système peut être décrit par le hamiltonien de *tight-binding* selon le formalisme de la second quantification[1]

$$H_0 = t \sum_{<x,y>} (c_x^\dagger c_y + c_y^\dagger c_x) \tag{1.1}$$

où nous n'avons pas considéré le spin des électrons.[2] Dans cette formule $c_x^\dagger, c_x$ représentent,

[1] Cela revient à considérer une matrice hors-diagonale sur $l^2(\mathbb{H}, \mathbb{C})$, ayant tous les éléments hors diagonale égaux à t.

[2] Une description plus générale doit tenir compte de la présence de champs extérieurs et de déformations

respectivement, l'opérateur de création et d'annihilation d'un électron en x, et $t \simeq -2.7eV$ est l'amplitude de saut des électrons. La notation $< x, y >$ indique que la somme est effectuée uniquement par rapport aux sites adjacents.

Supposons que le réseau Λ soit engendré par les vecteurs

(1.2) $$a_1 = \sqrt{3} l e_x, \qquad a_2 = \frac{l}{2}\left(\sqrt{3}e_x + 3e_y\right),$$

où $l = 0{,}142nm$ est la longueur des liens de carbone, et soient

(1.3) $$\delta_{1,2} = \frac{l}{2}\left(\pm\sqrt{3}e_x + e_y\right), \qquad \delta_3 = -le_y$$

le vecteurs qui connectent les sommets adjacents des deux réseaux Alors le hamiltonien

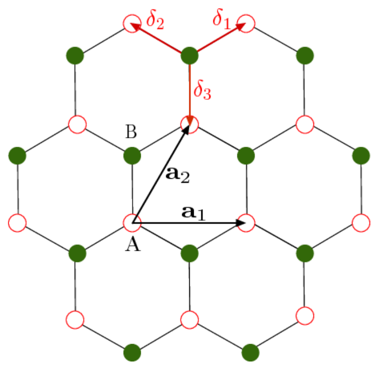

Figure 1.1. La structure en nid d'abeille du graphène [39].

(1.1) devient

(1.4) $$H_0 = \sum_{r \in A} \sum_{\alpha=1}^{3} \left(c_B^\dagger(r+\delta_\alpha)c_A(r) + c_A^\dagger(r)c_B(r+\delta_\alpha)\right).$$

On peut diagonaliser (1.4) à l'aide de la tranformation de Fourier

(1.5) $$c_j(r) = \frac{1}{\sqrt{N}} \sum_{k \in \mathcal{B}} e^{-ik\cdot r} c_j(k), \qquad j = A, B,$$

du réseau. Cela consiste à rajouter dans l'hamiltonien (1.1) un terme du type $U\sum_x \left(n_{x,\uparrow} - \frac{1}{2}\right)\left(n_{x,\downarrow} - \frac{1}{2}\right)$ qui répresente une intéractions localisé et un terme de déformation $\sum_{<x,y>} F(t_{xy})$. Dans la formule, $n_{x,\sigma}$ est l'opérateur qui compte les electrons dans le site x avec spin σ. On peut supposer que le coefficient t dépende des sites aussi: $t = t_{x,y}$. Dans le cadre de ce type de modèle, Frank et Lieb [58] ont récemment classifié les configurations possibles pour le réseau. On rémarque que en presence d'un champ magnétique on a $t \in \mathbb{C}$ et $t(c_x^\dagger c_y + c_y^\dagger c_x) \mapsto (tc_x^\dagger c_y + t^* c_y^\dagger c_x)$.

et cela donne

$$
\begin{aligned}
H_0 &= \sum_{k\in\mathcal{B}} \left(t \sum_{\alpha=1}^{3} \left(c_B^\dagger(k) e^{ik\cdot\delta_\alpha} c_A(k) + c_A^\dagger(k) e^{-ik\cdot\delta_\alpha} c_B(k) \right) \right) \\
&= \sum_{k\in\mathcal{B}} \begin{pmatrix} c_A^\dagger(k), & c_B^\dagger(k) \end{pmatrix} \begin{pmatrix} 0 & t\sum_{\alpha=1}^{3} e^{-ik\cdot\delta_\alpha} \\ t\sum_{\alpha=1}^{3} e^{ik\cdot\delta_\alpha} & 0 \end{pmatrix} \begin{pmatrix} c_A(k) \\ c_B(k) \end{pmatrix}
\end{aligned} \tag{1.6}
$$

où l'on a adopté cette notation pour remarquer qu'il s'agit d'un opérateur autoadjoint hors-diagonale. Donc la matrice qui apparaît dans la formule (1.6) peut s'écrire en fonction des matrices de Pauli comme

$$
h(k) := \begin{pmatrix} 0 & t\sum_{\alpha=1}^{3} e^{-ik\cdot\delta_\alpha} \\ t\sum_{\alpha=1}^{3} e^{ik\cdot\delta_\alpha} & 0 \end{pmatrix} = d_1(k)\sigma_1 + d_2(k)\sigma_2, \qquad k \in \mathcal{B}. \tag{1.7}
$$

Les fonctions $d_1(k), d_2(k)$ sont à valeurs réelles et satisfont

$$
d_1(k) + id_2(k) = t\sum_{\alpha=1}^{3} e^{ik\cdot\delta_\alpha}. \tag{1.8}
$$

Le spectre en énergie des électrons est donc donné par le spectre de la matrice qui apparaît dans (1.6)

$$
E_\pm(k) = \pm\sqrt{d_1^2(k) + d_2^2(k)}, \qquad k \in \mathbb{R}^2. \tag{1.9}
$$

La fonction E_- décrit la bande de valence du graphène et E_+ correspond à la bande de conduction. Les deux bandes se touchent dans les points $k \in \mathcal{B}$ tels que

$$
(d_1(k), d_2(k)) = 0.
$$

Un calcul direct montre qu'il y a deux points non équivalents (*Dirac points*) dans l'éspace dual

$$
k = \pm K = \pm\frac{4\pi}{3\sqrt{3}l} e_x. \tag{1.10}
$$

au sens où les autres solutions sont obtenues en appliquant les translations du réseau dual à $\pm K$. L'opérateur de Dirac apparaît dans cette description, si l'on développe le hamiltonien $H(k)$ au premier ordre autour des points $\pm K$.

Soit $k = \pm K + q$, avec $|q|l \ll 1$ où $q = q_x e_x + q_y e_y$ est une petite perturbation de $\pm K$. On réécrit les opérateurs de création/annihilation $c_{A\pm K}(q) = c_A(\pm K + q)$. Au premier ordre autour de $k = \xi K$ ($\xi = \pm 1$) on trouve

$$H_0^{(\xi K)} = v_F \sum_k \begin{pmatrix} c^\dagger_{A\xi K}(k), & c^\dagger_{B\xi K}(k) \end{pmatrix} \begin{pmatrix} 0 & \xi q_x - i q_y \\ \xi q_x + i q_y & 0 \end{pmatrix} \begin{pmatrix} c_{A\xi K}(k) \\ c_{B\xi K}(k) \end{pmatrix} \tag{1.11}$$

où $v_F = -3lt/2 \simeq 10^6 m.s^{-1} \simeq c/300$ est la vitesse de Fermi. On voit donc qu'autour des *points de Dirac* les électrons sont décrits par deux copies de l'operateur de Dirac bidimensionnel (voir Chapitre 2).

Si l'on adopte la notation

$$(c^\dagger_j(q))_{j=1}^4 = (c^\dagger_{A+K}(q), c^\dagger_{B+K}(q), c^\dagger_{B-K}(q), c^\dagger_{A-K}(q)),$$

on peut réécrire le hamiltonien linéarisé sous la forme

$$H_0 = \sum_q \sum_{j,k=1}^4 c^\dagger_j(q)[v_F \sigma_3 \otimes (\boldsymbol{\sigma} \cdot q)]_{j,k} c_k(q). \tag{1.12}$$

En général, au niveau de Fermi, les électrons sont décrits par une fonction d'onde à valeur dans $\mathbb{C}^4 = \mathbb{C}^2 \otimes \mathbb{C}^2$. Néanmoins, on verra dans la suite que si un électron est concentré en fréquence autour d'un seul des deux points $\pm K$, on peut se limiter à considerer des fonction à valeur dans $\mathbb{C}^2$ et donc tout simplement l'opérateur de Dirac en 2D.

Remark 1.1. Dans le cadre de modèles relativistes, la fonction d'onde d'un électron est à valeurs dans $\mathbb{C}^4$ (en dimension 3) car cela permet de décrire de façon naturelle son spin et de tenir compte de la presence de son antiparticule, le positron [118, 92]. Dans le cas du graphène, par contre, le fait d'avoir un spineur à valeur dans $\mathbb{C}^4 = \mathbb{C}^2 \otimes \mathbb{C}^2$ correspond au fait que le réseau hexagonal du cristal est donné par la superposition de deux réseaux triangulaires inéquivalents et la même chose est vraie pour le réseau dual. Donc il y a $4 = 2 \times 2$ degré de liberté pour les électrons. De plus, comme on l'a déjà remarqué, il n'y a pas d'interpretation des deux parties du spectre de l'opérateur de Dirac en termes de particules/antiparticules, mais elles représentent plutôt les bandes de conduction/valence du matériau.

1.2 L'opérateur de Dirac dans les structures *en nid d'abeille*

1.2.1 Opérateurs de Schrödinger et potentiels *en nid d'abeille*

Nous avons vu au paragraphe précédent que la structure d'une feuille de graphène est celle d'un réseau hexagonal, d'une structure *en nid d'abeille*. Au niveau macroscopique, on peut décrire le comportement des électrons par un opérateur de Schrödinger périodique

$$-\Delta + V(x), \qquad x \in \mathbb{R}^2, \tag{1.13}$$

où le potentiel $V : \mathbb{R}^2 \to \mathbb{R}$ doit avoir la symétrie du réseau, afin de tenir compte de la structure cristalline sous-jacente, comme d'habitude en physique du solide [104, 76]. Donc le comportement des électrons, en absence d'interactions, sera décrit par l'équation de Schrödinger linéaire suivante:

$$i\partial_t u = (-\Delta + V(x))\, u =: H_V u, \qquad u : \mathbb{R}_t \times \mathbb{R}^2_x \longrightarrow \mathbb{C}. \tag{1.14}$$

En particulier, les propriétés du propagateur $e^{-iH_V t}$ sont directement liées aux propriétés spectrales de l'opérateur H_V qui dépendent elles-mêmes des symètries du réseau. Le définition suivante formalise l'idée d'un potentiel qui a les symétries du réseau hexagonal.

Definition 1.2. On appelle un potentiel $V \in C^\infty(\mathbb{R}^2)$ *potentiel en nid d'abeille* (*honeycomb potential*) [56], s'il existe $x_0 \in \mathbb{R}^2$ tel que $\tilde{V}(x) = V(x - x_0)$ a les proprietés suivantes:

1. $\tilde{V}$ est périodique par rapport à Λ, c'est à dire, $\tilde{V}(x+v) = \tilde{V}(x)$, $\forall x \in \mathbb{R}^2, \forall v \in \Lambda$;
2. $\tilde{V}$ est paire: $\tilde{V}(-x) = \tilde{V}(x)$, $\forall x \in \mathbb{R}^2$;
3. $\tilde{V}$ est invariant par rapport à la rotation de $\frac{2\pi}{3}$ (au sens antihoraire)

$$\mathcal{R}[\tilde{V}](x) := \tilde{V}(R^* x) = \tilde{V}(x), \forall x \in \mathbb{R}^2,$$

   où R est la matrice de rotation correspondante:

$$R = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}. \tag{1.15}$$

Dans la suite on prend $x_0 = 0$ pour simplifier les notations.

Remark 1.3. (Quelques exemples de potentiels en nid d'abeille [56])

1. **Potentiels "atomiques"**: Soit $\mathbb{H} = (A + \Lambda) \cup (B + \Lambda)$ un réseau hexagonal (voir fig.1.1). On considére une fonction radiale $V_0 \in C^\infty(\mathbb{R}^2)$ et qui décroît rapidement à l'infini (avec une vitesse polynômiale, par example) et qui représente le potentiel engendré par un noyau situé sur un sommet du réseau. Le potentiel

$$V(x) = \sum_{y \in \mathbb{H}} V_0(x - y)$$

est donc donné par la superposition des potentiels atomiques. On peut vérifier que $V(x)$ est un potentiel en nid d'abeille (Def.1.2).

2. **Réseaux optiques:** L'enveloppe ψ du champ électrique d'un faisceau de lumière monochromatique qui se propage dans un milieu diélectrique peut être décrite par une équation de Schrödinger. Plus précisement, si l'on note z la direction de propagation du faisceau et on suppose que l'indice de réfraction du milieu varie uniquement dans les diréctions transversales (x, y), la fonction ψ est une solution de

   $$i\partial_z \psi = (-\Delta + V(x,y))\,\psi \tag{1.16}$$

   Dans ce cas le potentiel en nid d'abeille est engendré grâce à des techniques d'interférence de faisceaux de lumière [98]. Typiquement, le potentiel $V(x, y)$ est de la forme

   $$V(x,y) \simeq V_0\left(\cos(k_1\cdot(x,y)) + \cos(k_1\cdot(x,y)) + \cos((k_1+k_2)\cdot x)\right), \quad V_0 \in \mathbb{R}, k_1, k_2 \in \mathbb{R}^2. \tag{1.17}$$

Pour chaque $k \in \mathbb{R}^2$ fixé on considère le problème aux valeurs propres avec conditions de *pseudo-périodicité* suivant (voir [56] and [104, Sec. XIII.16])

$$\begin{cases} H_V\Phi(x;k) = \mu(k)\Phi(x;k), & x \in \mathbb{R}^2 \\ \Phi(x+v;k) = e^{ik\cdot v}\Phi(x;k), & v \in \Lambda. \end{cases} \tag{1.18}$$

Si on pose $\Phi(x;k) = e^{ik\cdot x}p(x;k)$, on peut aisément vérifier que $p(x;k)$, $k \in \mathcal{B}$, est périodique et est une solution du problème equivalent

$$\begin{cases} H_V(k)p(x;k) = \mu(k)p(x;k), & x \in \mathbb{R}^2 \\ p(x+v;k) = p(x;k), & v \in \Lambda. \end{cases} \tag{1.19}$$

où

$$H_V(k) := (\nabla + ik)^2 + V(x).$$

Remark 1.4. Les fonction propres $\Phi(x;k)$ sont de classe C^∞ d'après la théorie de la régularité élliptique classique [63].

Pour tout $k \in \mathcal{B}$, la résolvante de $H_V(k)$ est compacte et donc le spectre de l'opérateur est discret et réel et s'accumule à $+\infty$:

$$\mu_1(k) \leqslant \mu_2(k) \leqslant \ldots \leqslant \mu_j(k) \leqslant \ldots \uparrow +\infty. \tag{1.20}$$

Si on fixe $n \in \mathbb{N}$ on dit que la fonction $k \mapsto \mu_n(k)$ est la n-ième *bande de dispérsion* de l'opérateur H_V et on appelle n-ième *onde de Bloch* la fonction $\Phi_n(x,k)$. Le spectre de H_V peut avoir des lacune (*gaps*). Il s'obtient comme union des graphes des bandes de l'opérateur

$$\mathrm{Spec}(H_V) = \bigcup_{n\in\mathbb{N}} \mu_n(\mathcal{B}), \tag{1.21}$$

et il est donné par l'union des intervalles $\mu_n(\mathcal{B})$.

Les ondes de Bloch forment un système complet, au sens où pour tout $f \in L^2(\mathbb{R}^2)$

$$f(x) - \sum_{1\leqslant n\leqslant N} \int_{\mathcal{B}} \langle \Phi_n(\cdot,k), f(\cdot)\rangle_{L^2(\mathbb{R}^2)} \Phi_n(x;k)dk \longrightarrow 0 \tag{1.22}$$

dans $L^2(\mathbb{R}^2)$, pour $N \longrightarrow +\infty$ [56, 104]. Le problème de Cauchy

$$\begin{cases} i\partial_t u(t,x) = H_V u(t,x), & (t,x) \in \mathbb{R}\times\mathbb{R}^2, \\ u(0,x) = u_0(x) \in L^2(\mathbb{R}^2), \end{cases} \tag{1.23}$$

admet la solution

$$e^{-iH_V t}u_0 = \sum_{n\in\mathbb{N}} \int_{\mathcal{B}} e^{-i\mu_n(k)} \langle \Phi_n(\cdot,k), u_0(\cdot)\rangle_{L^2(\mathbb{R}^2)} \Phi_n(x,k)dk. \tag{1.24}$$

Donc c'est évident que la dynamique (1.24) est influencée par le comportement des fonctions $\mu_n(\cdot)$, $n \in \mathbb{N}$.

Les propriétés spectrales des structures en nid d'abeille on été largement étudiées dans la littérature, notamment dans le régime limite de *tight-binding* ou dans le cas de potentiels concentré sur des graphes [79, 123] et dans le regime de potentiels faibles avec arguments pertubatifs [2, 69, 66]. Un résultat général concernant l'existence de croisements coniques pour les bandes de dispersion d'opérateurs de Schrödinger en nid d'abeille a été prouvé par Fefferman and Weinstein dans [56].

Soit V un potentiel en nid d'abeille (Def.1.2) et soit K un sommet de la zone de Brillouin du réseau $\mathbb{H}^*$. On considère l'espace des fonctions L^2 K-pseudopériodiques, L^2_K défini par

$$L^2_K = \left\{ f \in L^2(\Omega) : f(x+v) = e^{K\cdot v} f(x), \forall v \in \Lambda \right\}. \tag{1.25}$$

où Ω est la cellule élémentaire du réseau $\mathbb{H}$.

Si $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$, on pose

$$\mathcal{R}[f](x) := f(R^* x), \qquad x \in \mathbb{R}^2, \tag{1.26}$$

et R est la matrice (1.15). Le laplacien étant invariant par rotation et le potentiel étant $\mathcal{R}$-invariant, on peut montrer la relation de commutation suivante

$$[\mathcal{R}, H_V(K)] = 0. \tag{1.27}$$

De plus, soient $1, \tau = \exp 2\pi i/3, \overline{\tau}$ les valeurs propres de $\mathcal{R}$, on peut en conséquence décomposer L^2_K comme somme directe des sous-espaces spectrals de $\mathcal{R}$

$$L^2_K = L^2_{K,1} \oplus L^2_{K,\tau} \oplus L^2_{K,\overline{\tau}}, \tag{1.28}$$

où

$$L^2_{K,\sigma} := \left\{ f \in L^2_K : \mathcal{R}f = \sigma f \right\}, \qquad \sigma = 1, \tau, \overline{\tau}. \tag{1.29}$$

Definition 1.5. (*Points de Dirac / Dirac points*, [56]) Soit V un potentiel en nid d'abeille et $\mathcal{B}$ la zone de Brillouin du réseau hexagonal sous-jacent. On dit que $K \in \mathcal{B}$ est un *point de Dirac* si les propriétés suivantes sont verifiées.

Il existe $n \in \mathbb{N}$, $\mu_* \in \mathbb{R}$ et $\lambda, \delta > 0$ tels que:

1. $\dim \ker (H_V(K) - \mu_*) = 2$,
2. $\ker (H_V(K) - \mu_*) = \operatorname{span} \{\Phi_1(x, K), \Phi_2(x, K)\}$, où $\Phi_1 \in L^2_{K,\tau}$ et $\Phi_2 = \overline{\Phi_1(-x)} \in L^2_{K,\overline{\tau}}$,
3. Il existe deux fonctions Lipschitz $E_\pm : U_\delta \to \mathbb{R}$, où $U_\delta := \left\{ y \in \mathbb{R}^2 : |y| < \delta \right\}$, telles que pour $|k - K| < \delta$,

$$\begin{cases} \mu_{n+1}(k) - \mu(K) = |\lambda_\#||k - K| \left(1 + E_+(k - K)\right), \\ \mu_n(k) - \mu(K) = -|\lambda_\#||k - K| \left(1 + E_-(k - K)\right). \end{cases} \tag{1.30}$$

avec $E_\pm(y) = O(|y|)$, pour $|y| \to 0$.

La constante $\lambda_\# \in \mathbb{C} \setminus \{0\}$ dépend du potentiel V [56].

Essentiellement, un point de Dirac est un point de la zone de Brillouin $K \in \mathcal{B}$ tel que l'hamiltonien $H_V(K)$ ait une valeur propre double (1.19) et cela correspond à deux bandes μ_n, μ_{n+1} qui se touchent en un point tel que, au premier ordre, le graphe de la relation de dispersion soit un cône. En particulier, les bandes sont seulement des fonctions Lipschitz autour de ces points coniques.

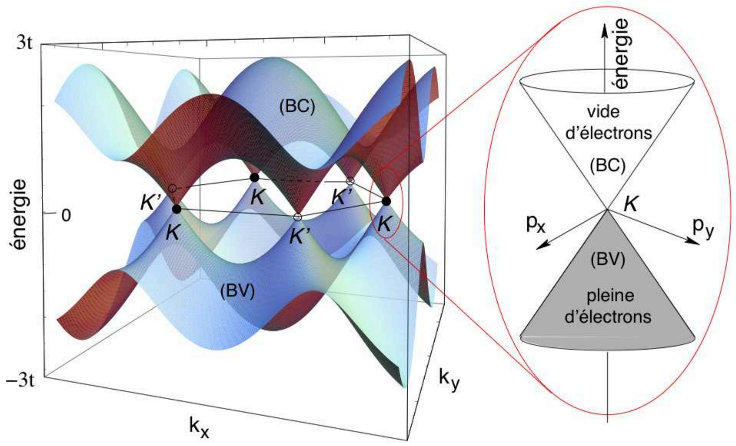

Figure 1.2. Une représention des cones de Dirac aux sommets de la zone de Brillouin [61].

Remark 1.6. La propriété (1.30) explique pourquoi ces points sont appelée points de Dirac. D'après la formule (2.16) il est évident que pour le cas à masse nulle, la relation de dispersion de l'opérateur de Dirac donne exactement un cône.

Dans [56] Fefferman and Weinstein ont démontré que les opérateurs de Schrödinger en nid d'abeille possèdent des points de Dirac dans leur spectre, sous des hypothèses très générales.

Theorem 1.7. *(Existence des points de Dirac, [56]) Soit $V(x)$ un potentiel en nid d'abeille et supposons que le coefficient de Fourier de V, $V_{1,1}$ ne soit pas nul;*

$$V_{1,1} := \int_{\Omega} e^{-i(k_1+k_2)\cdot x} V(x)\, dx \neq 0. \tag{1.31}$$

Considérons la famille de hamiltoniens en nid d'abeille suivante

$$H^{\varepsilon} := -\Delta + \varepsilon V(x), \qquad \varepsilon > 0, \tag{1.32}$$

Il existe un ensemble fermé dénombrable $\mathcal{C} \subset \mathbb{R}$ tel que pour tout $\varepsilon \notin \mathcal{C}$, les sommets de la zone de Brillouin $\mathcal{B}$ sont des points de Dirac au sens de la définition 1.5.

Plus précisement, on peut montrer qu'il existe $\varepsilon_0 > 0$ tel que $\forall \varepsilon \in (-\varepsilon_0, \varepsilon_0) \setminus \{0\}$

i) si $\varepsilon V_{1,1} > 0$, la 1ère et la 2ème bande ont un croisement conique,

ii) si $\varepsilon V_{1,1} < 0$, la 2ème et la 3ème bande ont un croisement conique.

et donc $\mathcal{C} \cap (-\varepsilon_0, \varepsilon_0) = \emptyset$. L'existence de l'ensemble $\mathcal{C}$ est due à des obstructions topologiques [56]. Une question très importante au niveau théorique et pour les applications et celle de la stabilité des point de Dirac. Pour le graphène, par example, il est bien connu dans la littérature physique que la symètries fondamentale qui protège les cônes de Dirac est la symètrie $\mathcal{PT}$, c'est à dire la composition de la symètrie par renversement du temps et de la parité spatiale [39]. Et donc une perturbation qui respecte cette symétrie peut déformer le cônes, mais en général, cela ne suffit pas pour ouvrir un *gap* dans le spectre. Pourtant, un mécanisme pour l'ouverture d'un gap au niveau de Fermi par déformation du réseau a été recemment proposé dans la littérature [87]. On peut ouvrir un *gap* dans le spectre si l'on tient compte du spin ou si l'on rajoute un champ magnétique [68, 74]. Les mécanisme d'ouverture d'un gap au niveau de Fermi ont été classifiés et peuvent être décrits en termes d'un hamiltonien efficace qui fait intervenir l'opérateur de Dirac [39].

Dans [56] l'effet d'une petite perturbation sur les points de Dirac d'un opérateur de Schrödinger en nid d'abeille a été étudié.

Remark 1.8. Dans le cadre de la mécanique quantique non relativiste, les opérateurs de parité (par rapport à l'origine) et de renversement du temps sont donnés, respectivement, par

$$\mathcal{P}u(x) = u(-x), \qquad \mathcal{T}u(x) = \overline{u(x)}, \tag{1.33}$$

où $u : \mathbb{R}^d \longrightarrow \mathbb{C}$ est la fonction d'onde de la particule [107].

Soit $V(x)$ un potentiel en nid d'abeille qui a des points de Dirac dans son spectre.

Theorem 1.9. *(Stabilité des points de Dirac,[56]) Soit $W \in C^\infty(\mathbb{R}^2; \mathbb{R})$ un potentiel pair, Λ-invariant, mais pas forcement $\mathcal{R}$-invariant (voir def. 1.5). Considérons l'opérateur*

$$H(\eta) := -\Delta + V(x) + \eta W(x), \qquad \eta \in \mathbb{R}. \tag{1.34}$$

1. *Il existe $\eta_1 > 0$ et des fonctions de classe C^∞*

$$\begin{cases} \eta \mapsto \mu^{(\eta)} = \mu(K) + O(\eta) \in \mathbb{R}, \quad \eta \mapsto K^{(\eta)} = K + O(\eta) \in \mathcal{B}, \\ \eta \mapsto \phi_j^{(\eta)}(x; K^{(\eta)}) = \phi_j(x) + O(\eta) \in L^2(\mathbb{R}/\Lambda). \end{cases} \tag{1.35}$$

définies sur $\{|\eta| < \eta_1\}$, tels que $\mu^{(\eta)}$ est une valeur propre double pour $H(\eta)$ dans $L^2_{K^{(\eta)}}$ avec sous-espace associé engendré par

$$\left\{\Phi_1^{(\eta)}, \Phi_2^{(\eta)}\right\} = \left\{e^{iK^{(\eta)}\cdot x}\phi_1^{(\eta)}(x; K^{(\eta)}), e^{iK^{(\eta)}\cdot x}\phi_2^{(\eta)}(x; K^{(\eta)})\right\}.$$

2. *L'operateur $H(\eta)$ a un croisement conique de ses bandes de dispersion autour des points $K^{(\eta)} = K + O(\eta)$, et les bandes qui se touchent sont données par des fonctions $\mu_n^{(\eta)}(k), \mu_{n+1}^{(\eta)}(k)$ définies autour de $K^{(\eta)}$*
(1.36)
$$\begin{cases} \mu_{n+1}^{(\eta)}(k) - \mu(K^{(\eta)}) = \eta b^{(\eta)} \cdot (k - K^{(\eta)}) + \left(\mathcal{Q}(k - K^{(\eta)})\right)^{\frac{1}{2}} \left(1 + E_+^{(\eta)}(k - K^{(\eta)})\right) \\ \mu_n^{(\eta)}(k) - \mu(K^{(\eta)}) = \eta b^{(\eta)} \cdot (k - K^{(\eta)}) - \left(\mathcal{Q}(k - K^{(\eta)})\right)^{\frac{1}{2}} \left(1 + E_-^{(\eta)}(k - K^{(\eta)})\right). \end{cases}$$
où $b^{(\eta)} \in \mathbb{R}^2$ et la forme quadratique $\mathcal{Q}^{(\eta)}(\cdot)$ sont des fonctions de classe C^∞ de η. Enfin,
$$(|\lambda_\#|^2 - C|\eta|)\left(y_1^2 + y_2^2\right) \leqslant \mathcal{Q}^{(\eta)}(y) \leqslant \left(|\lambda_\#|^2 + C|\eta|\right)(y_1^2 + y_2^2)$$
pour $|\eta| \leqslant \eta_1$ et $y = (y_1, y_2) \in \mathbb{R}^2$, avec $0 < \eta_1 \ll 1$. De plus on a $\left|E_\pm^{(\eta)}(y)\right| \leqslant C|y|$, pour $|\eta| \leqslant \eta_1, |y| \leqslant \delta$, où $0 < \delta \ll 1$ et $C > 0$.

Donc le théoreme dit que si l'on rajoute une petite perturbation qui n'est pas forcément $\mathcal{R}$-invariante mais qui respecte la symétrie de parité et le renversement du temps (le potentiel W est réel) alors l'opérateur correspondant a toujours des croisements coniques, mais qui ne sont plus forcément situés aux sommets de la zone de Brillouin. De plus, la valeur de l'énergie qui correspond au sommet du cône peut changer, et en général elle est du type $\mu(K) + O(\eta)$, où η est la taille de la perturbation. En particulier, on peut montrer que si W est un potentiel en nid d'abeille on a $K^{(\eta)} = K$.

Remark 1.10. Soit $W \in C^\infty(\mathbb{R}^2)$, Λ-périodique mais pas forcément tel que $W(-x) = W(x), \forall x \in \mathbb{R}^2$, et donc qui brise la parité. Typiquement, dans ce cas on a

$$\langle \Phi_1, W\Phi_1 \rangle \neq \langle \Phi_2, W\Phi_2 \rangle. \tag{1.37}$$

Sous cette hypothèse on peut montrer qu'il n'y a plus de croisement conique, car les deux valeurs propres correspondantes deviennent simples et donc on ouvre un trou spectrale, et les bandes de dispersion sont de classe C^∞ [56]. Dans ce cas, le gap corréspond à un terme de masse constante dans l'opérateur de Dirac efficace [110].

1.2.2 Paquets d'onde et points de Dirac

Dans la section précédente nous avons énoncé le résultat de Fefferman and Weinstein [56] qui montre que les opérateurs de Schrödinger en nid d'abeille ont des cônes de Dirac dans le spectre, sous des hypothèses très générales. Il est donc naturel que l'évolution d'un paquet d'onde concentré autour d'un point de Dirac soit décrite par une équation de Dirac et que cette approximation soit consistante au moins pour un temps fini, lorsque le paquet d'onde reste concentré autour du croisement conique. De façon générale, la dynamique pour des données initiales concentrées (en fréquence) autour d'un point dans l'espace dual est décrite, au moins localement en temps, par un opérateur efficace qui dépend des proprietés géométriques des bandes, comme montré par exemple dans [11, 70].

Soit $u_0 = u_0^\varepsilon$ un paquet d'onde concentré autour d'un point de Dirac, et qui est donc une modulation d'ondes de Bloch:

$$u_0^\varepsilon(x) = \sqrt{\varepsilon}(\alpha_{0,1}(\varepsilon x)\Phi_1(x) + \alpha_{0,2}(\varepsilon x)\Phi_2(x)), \qquad x \in \mathbb{R}^2, \varepsilon > 0, \tag{1.38}$$

où les fonctions $\Phi_j(x) := \Phi_j(x, K), j = 1{,}2$ sont les ondes de Bloch au point de Dirac $k = K$ (1.18), et les $\alpha_{0,j}$ sont des amplitudes (complexes) à déterminer. On s'attend à ce que, au premier ordre en ε, la solution de (1.14) avec donnée initiale (1.38) soit encore une modulation d'ondes de Bloch, avec des coefficients qui dépendent du temps:

$$u^\varepsilon(t,x) \underset{\epsilon \to 0^+}{\sim} \sqrt{\varepsilon}\left(\alpha_1(\varepsilon t, \varepsilon x)\Phi_1(x) + \alpha_2(\varepsilon t, \varepsilon x)\Phi_2(x) + \mathcal{O}(\varepsilon)\right). \tag{1.39}$$

Remark 1.11. Le facteur $\sqrt{\varepsilon}$ dans les formules (1.38,1.39) n'a aucun influence sur le résultat, évidemment, car il s'agit d'une équation linéaire. Le seul effet de ce changement d'échelle est de normaliser la norme L^2 des solutions.

Dans [57] Fefferman and Weinstein ont démontrer le résultat suivant

Theorem 1.12. *(Linear Dirac dynamics in honeycomb structures,[57]) On fixe $\rho > 0$,$\delta > 0$,$N \in \mathbb{N}$. L'équation de Schrödinger $i\partial_t u = (-\Delta + V)u$ admet une seule solution, qui est de la forme*

$$u^\varepsilon(t,x) = e^{-i\mu_* t}\left(\sum_{j=1}^{2} \sqrt{\varepsilon}\psi_j(\varepsilon t, \varepsilon x)\Phi_j(x) + \eta^\varepsilon(t,x)\right) \tag{1.40}$$

with $u^\varepsilon(0,x) = u_0^\varepsilon(x), \eta^\varepsilon(0,x) = 0$. Pour tout $|\beta| \leqslant N$ on a

$$\sup_{0 \leqslant t \leqslant \rho\varepsilon^{-2+\delta}} \|\partial_x^\beta \eta^\varepsilon(t,x)\|_{L_x^2(\mathbb{R}^2)} \xrightarrow{\varepsilon \to 0} 0. \tag{1.41}$$

Les coefficients $(\psi_1, \psi_2)^T$ satisfont l'équation de Dirac suivante

$$i\partial_t \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 & \overline{\lambda}(\partial_1 + i\partial_2) \\ \lambda(\partial_1 - i\partial_2) & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad 0 \neq \lambda \in \mathbb{C}, \tag{1.42}$$

avec données initiales $\begin{pmatrix} \psi_1(0,x) \\ \psi_2(0,x) \end{pmatrix} = \begin{pmatrix} \psi_{1,0}(x) \\ \psi_{2,0}(x) \end{pmatrix} \in [\mathcal{S}(\mathbb{R}^2)]^2$.

Remark 1.13. Le résultat a été démontré pour des données initiales de classe de Schwartz, mais Fefferman and Weinstein indiquent que c'est seulement une hypothèse technique.

Le théorème ci-dessus montre donc qu'effectivement si l'on prend des données initiales qui sont des modulation d'ondes de Bloch pour $k = K$, la solution de (1.14) reste une modulation d'ondes de Bloch, plus une erreuer qui reste petit sur un interval de l'ordre $\varepsilon^{-2+\delta}$, pour tout $\delta > 0$. Ici $\varepsilon > 0$ répresent l'échelle de variation/concentration des données initiales (1.38).

L'idée de la preuve du Théor ème 1.12 consiste à faire un ansatz du type (1.40) pour la solution de (1.14). Cela donne une equation pour l'erreur η^ε, qui peut être estimée avec la formule de Duhamel en décomposant le propagateur $e^{it(-\Delta+V)}$ de façon à analyser séparément les terme supportés (en fréquence) autour et loin de K. L'équation de Dirac (1.42) apparait donc comme condition de non-résonance qui permet de contrôler les termes supportés autour de K et de prouver l'estimation (1.41) [57].

1.2.3 Échantillons de graphène

Afin d'étudier les propriétés électroniques du graphène il est intéressant de tenir compte des dimensions finies des échantillons. Cela mène naturellement à considérer des conditions au bord (locales) pour l'opérateur de Dirac efficace[3]. Les conditions acceptables doivent respecter le principe de conservation du courant et la symétrie par renversement du temps [9, 122]. Les conditions plus utilisées dans la littérature physique sont les conditions *zigzag*, *armchair* et *infinite mass*. Les deux premières sont liées à la géométrie du bord de l'échantillon de graphène, tandis que la dernières correspondent à rajouter un terme de

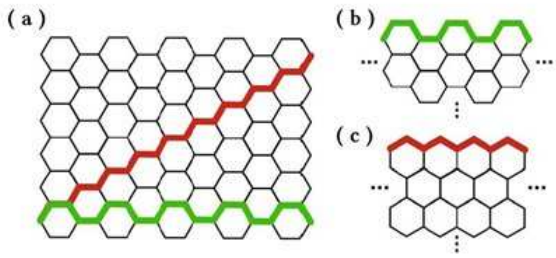

Figure 1.3. Bord *zigzag* (rouge) et *armchair* (vert), pour un échantillon de graphène [109].

[3]Des conditions locales au bord pour un opérateur de Dirac avaient déjà été considérées dans la littérature physique pour des raisons théoriques [22].

masse "infinie" dans le hamiltonien efficace (voir le lemme 2.9). La condition *infinite mass* est physiquement réalisée à partir de la condition *zigzag*, par des différences de potentiel opposées sur les sommets des deux réseaux triangulaires qui constituent la structure en nid d'abeille du graphène [9]. La condition *armchair* est réalisée uniquement pour un ensemble discret d'orientations du bord de l'échantillon, dans les autres cas la condition étant de type *zigzag*. Vu que pour cette dernière il n'y a pas de trou spectrale on en déduit que dans ce cas le graphène se comporte génériquement comme un métal [59]. Le conditions *zigzag* et *infinite mass* ont, au contraire, un gap dans le spectre, comme expliqué dans la section 2.2. En imposant la conservation du courant et la symétrie par renversement du temps, on trouve una famille de conditions linéaires au bord [9, 122]. Les conditions zigzag,armchair et infinite mass peuvent être décrites dans ce cadre, comme on verra dans la suite (section 2.2).

1.3 Graphes quantiques

Dans la literature on appelle *graphes quantiques* (*quantum graphs*) des graphes metriques (Figure 1.3) munis d'un opérateur différentiel defini sur chaque arête, identifié avec un segment ou une demi-droite. Afin d'avoir un opérateur auto-adjoint on doit imposer des conditions de raccordement sur les sommets du réseau. L'opérateur représent le hamiltonien du système, d'où le nom *graphes quantiques*. Des definitions et des références plus précises seront données dans la section 2.3.

Dans la littérature physique, le graphes quantiques ont été proposés pour decrire des systèmes qui peuvent être considerés essentiellement unidmensionnels. Dans ces cas le confinement des particules est realisé grâce à des potentiels de piégeage, qui justifient l'approximation de graphe. Dans le dernières années l'equation de Schrödinger suivante

$$i\frac{dv}{dt} = -\frac{d^2v}{dx^2} - |v|^{p-2}v, \qquad p \geqslant 2, \tag{1.43}$$

a été étudiée comme modele efficace pour décrire le comportement des condensés de Bose-Einstein dans des piégeages ramifiés, notamment dans le cas $p = 4$, voir e.g. [65]. En particulier, on peut s'interesser à l'éxistence de solutions stationnaires

$$v(t,x) = e^{-i\lambda t}u(x), \qquad \lambda \in \mathbb{R} \tag{1.44}$$

et donc à l'equation

$$-\frac{d^2u}{dx^2} - |u|^{p-2}u = \lambda u. \tag{1.45}$$

On cherche des solutions de (1.45) qui satisfont des conditions de raccordement sur le sommets du réseau, dont le plus utilisées sont le condition de type *Kirchoff* (voir la section 2.3).

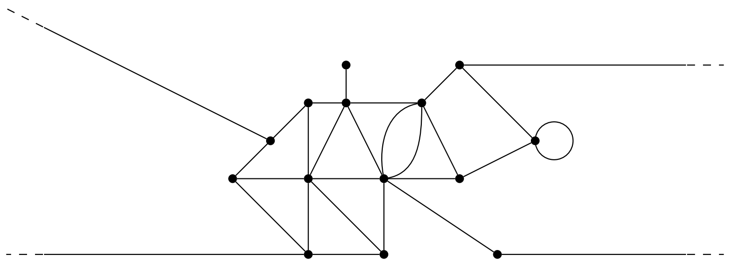

Figure 1.4. Un exemple de graphe non compacte $\mathcal{G}$.

Récemment des equations de Dirac non linéaires unidimensionnelles ont été proposés comme modele efficace pour des guides d'ondes [120, 121, 119]. Dans le papier [106] une équation de Dirac cubique sur un *3-star graph* (Figure 1.3) a été proposée, où l'on impose des conditions de type Kirchoff pour le spineur.

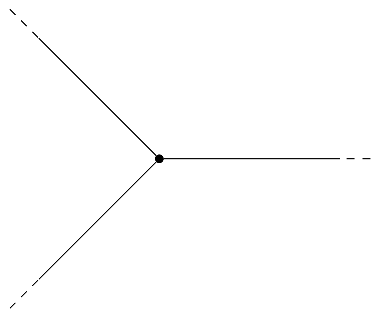

Figure 1.5. The infinite 3-star graph.

Dans les chapitres suivants on montrera que l'opérateur de Dirac avec ces conditions aux sommets est auto adjoint (section 2.3). Le chapitre 5 est consacrée à l'etude d'une famille d'équations de Dirac sur des graphes ayant une partie non compacte non triviale (*compact core*) $\mathcal{K} \subseteq \mathcal{G}$, sur laquelle la nonlinéaritée est définie. Notamment, on montrera l'existence d'une infinitée de solutions stationnaires et qu'elles convergent, dans un certain regime de paramètres, vers les solutions d'une équation de Schrödinger non linéaire.

Chapter 2

The Dirac operator in dimension one and two

In this section we quickly review Dirac's original argument which led to the equation which bears its name, in the attempt of describing the relativistic motion of spin-$\frac{1}{2}$ particles in $\mathbb{R}^3$. Our presentation is based on [118].

The derivation of the Dirac equation raised the question whether there exists a square root of the laplacian. Consider a particle in $\mathbb{R}^3$ with spin $\frac{1}{2}$. Denote by $m \geqslant 0$ its mass and by E and $\boldsymbol{p}$ its energy and momentum, respectively. Then, according to Special Relativity, the Hamiltonian of the particle is

$$E = \sqrt{c^2 p^2 + m^2 c^4}, \qquad p = |\boldsymbol{p}|. \tag{2.1}$$

The transition from classical to quantum mechanics is usually accomplished by substituting classical quantities with operators acting on the wavefunction of the particle, according to the prescription

$$E \longrightarrow i\hbar \frac{\partial}{\partial t}, \qquad \boldsymbol{p} \longrightarrow -i\hbar \nabla \tag{2.2}$$

Then the energy-momentum relation (2.1) gives the square-root Klein-Gordon equation for the wavefunction of the particle ψ

$$i\hbar \frac{\partial}{\partial t} \psi(t,x) = \left(\sqrt{-c^2 \hbar^2 \Delta + m^2 c^4} \right) \psi(t,x), \qquad t \in \mathbb{R}, x \in \mathbb{R}^3. \tag{2.3}$$

Here $\sqrt{-c^2 \hbar^2 \Delta + m^2 c^4}$ is the pseudo-differential operator of symbol $\sqrt{c^2 |\xi|^2 + m^2 c^4}$.

Dirac reconsidered the relation (2.1) and linearized it before applying the quantization rules (2.2). He wrote

$$E = c\sum_{j=1}^{3}\alpha_j p_j + \beta mc^2 = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2, \tag{2.4}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β have to be determined imposing (2.1). It turns out that $\boldsymbol{\alpha}$ and β must be anticommuting quantities, and they can be naturally assumed to be matrices $n \times n$ complex matrices. Comparing E^2 according to (2.1) and (2.4) one finds that the following relations must be satisfied

$$\begin{aligned} &\alpha_j\alpha_k + \alpha_k\alpha_j = 2\delta_{j,k}\mathbb{1}_n, \qquad j,k = 1,2,3,\\ &\alpha_j\beta + \beta\alpha_j = \mathbb{0}_n, \qquad j = 1,2,3,\\ &\beta^2 = \mathbb{1}_n. \end{aligned} \tag{2.5}$$

here $\delta_{j,k}$ is the Kronecker symbol and $\mathbb{0}_n$ and $\mathbb{1}_n$ are the zero and the unit n-dimensional matrix, respectively. Moreover, one looks for *hermitian* matrices α_j, β, as the resulting operator should be self-adjoint. The (minimal) dimension n of the matrices can be determined as follows. The relations (2.5) imply that

$$\operatorname{tr}\alpha_j = \operatorname{tr}\beta^2\alpha_j = -\operatorname{tr}(\beta\alpha_j\beta) = -\operatorname{tr}\alpha_j\beta^2 = -\operatorname{tr}\alpha_j = 0 \tag{2.6}$$

and thus the matrices α_j are traceless. On the other hand, there holds $\alpha_j^2 = \mathbb{1}_n$ and then n must be an even number. For $n = 2$ there are at most three linearly independent anticommuting matrices. Indeed, it can be easily checked that the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.7}$$

together with the unit matrix $\mathbb{1}_2$ form a basis in the space of hermitian 2×2 matrices. Then, in two dimensions there is no "rest energy" matrix β.

Passing to four dimensions, one can easily verify that the relations (2.5) are satisfied choosing the following block matrices

$$\alpha_j = \begin{pmatrix} \mathbb{0}_2 & \sigma_j \\ \sigma_j & \mathbb{0}_2 \end{pmatrix}, \qquad \beta = \begin{pmatrix} \mathbb{1}_2 & \mathbb{0}_2 \\ \mathbb{0}_2 & -\mathbb{1}_2 \end{pmatrix}. \tag{2.8}$$

This choice of matrices is known in the Physics literature as the *Dirac* or *standard representation* of the Dirac matrices. Other choices are possible, each having its own advantages.

Remark 2.1. This fact is related to an underlying algebraic structure. Indeed, Pauli matrices are the generators of a representation of the *Clifford algebra* of the three dimensional euclidean space, on the vector space $\mathbb{C}^4$. Thus different choices of the Dirac matrices correspond to unitarily equivalent representations. Those structures allow, more generally, to define the Dirac operators on suitable riemannian manifolds (the so-called *spin manifolds*). More details can be found e.g. in [73, 60].

Translating (2.4) using the quantization rules one obtains the Dirac equation

$$i\hbar\frac{\partial}{\partial t}\psi(t,x) = \mathcal{D}\psi(t,x) \tag{2.9}$$

where $\mathcal{D}$ is given by the matrix-valued differential expression

$$\mathcal{D} = -i\hbar c\boldsymbol{\alpha}\cdot\nabla + \beta mc^2 = \begin{pmatrix} mc^2\mathbb{1}_2 & -i\hbar c\boldsymbol{\sigma}\cdot\nabla \\ -i\hbar c\boldsymbol{\sigma}\cdot\nabla & -mc^2\mathbb{1}_2 \end{pmatrix} \tag{2.10}$$

where $\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)$. The Dirac operator acts on vector-valued functions, usually called *spinors*

$$\psi(t,x) = \begin{pmatrix} \psi_1(t,x) \\ \psi_2(t,x) \\ \psi_3(t,x) \\ \psi_4(t,x) \end{pmatrix} \in \mathbb{C}^4. \tag{2.11}$$

In space-dimension two and one, it is sufficient to use Pauli matrices and the minimal dimension such that the relations (2.5) are satisfied is $n = 2$ in both cases. Then the operator acts of $\mathbb{C}^2$-valued spinors. More precisely, in the two-dimensional case a common choice is

$$\mathcal{D} = -i\hbar c\left(\sigma_1\frac{\partial}{\partial x_1} + \sigma_2\frac{\partial}{\partial x_2}\right) + \sigma_3 mc^2. \tag{2.12}$$

In one dimension only two anticommuting matrices are needed. We will define the Dirac operator as follows

$$\mathcal{D} = -i\hbar c\sigma_1\frac{d}{dx} + mc^2\sigma_3. \tag{2.13}$$

In the next sections we will focus on Dirac operators in dimension one and two. We will describe different self-adjoint realizations as L^2- operators of the formal differential expressions (2.12,2.13), obtained imposing suitable boundary conditions. In the following we shall always use units where $\hbar = 1$ and $c = 1$. Except in Chapter 5 where we study the nonrelativistic limit ($c \to +\infty$) of solutions to Dirac equations on metric graphs.

2.1 The case of $\mathbb{R}^2$

In this section we follow again the presentation given in [118].

The Dirac operator can be easily analyzed using the Fourier transform[1] $\mathcal{F}$. In order to distinguish between the variabiles, we shall write

$$\mathcal{F}L^2(\mathbb{R}^2, dx)^2 = L^2(\mathbb{R}^2, dp)^2.$$

The latter is often called the *momentum space*. The key point, as usual, is that a matrix differential operator with constant coefficient in $L^2(\mathbb{R}^2, dx)^2$ is transformed by $\mathcal{F}$ into a matrix multiplication operator on the momentum space $L^2(\mathbb{R}^2, dp)^2$, which is much easier to analyze.

For the Dirac operator $\mathcal{D} = -i\,(\sigma_1 \partial_{x_1} + \sigma_2 \partial_{x_2}) + m\sigma_3$ one obtains

$$\left(\mathcal{F}\mathcal{D}\mathcal{F}^{-1}\right)(p) = h(p) = \begin{pmatrix} m & p_1 - ip_2 \\ p_1 + ip_2 & -m \end{pmatrix}. \tag{2.15}$$

For each $p \in \mathbb{R}^2$ the hermitian matrice $h(p)$ has eigenvalues

$$\lambda_1(p) = -\lambda_2(p) = \sqrt{|p|^2 + m^2}. \tag{2.16}$$

The matrix $h(p)$ is diagonalized by the unitary transformation

$$u(p) = a_+(p)\mathbb{1}_2 + a_-(p)\sigma_3 \frac{\boldsymbol{\sigma} \cdot p}{|p|}, \tag{2.17}$$

where

$$a_\pm(p) = \frac{1}{\sqrt{2}}\sqrt{1 \pm \frac{m}{\lambda(p)}}. \tag{2.18}$$

---

[1] We adopt the following convention

$$(\mathcal{F}\psi_k)(p) := \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{-ip\cdot x}\psi_k(x)\,dx, \qquad k = 1,2, \tag{2.14}$$

in the definition of the transform.

One can check that there holds

$$u(p)h(p)u^{-1}(p) = \sigma_3\lambda(p) = \begin{pmatrix} \lambda(p) & 0 \\ 0 & -\lambda(p) \end{pmatrix}. \tag{2.19}$$

Then combining (2.15) and (2.19) we conclude that the unitary transformation

$$\mathcal{W} = u\mathcal{F} \tag{2.20}$$

converts the Dirac operator $\mathcal{D}$ into the operator of multiplication by the matrix[2]

$$\left(\mathcal{W}\mathcal{D}\mathcal{W}^{-1}\right)(p) = \sigma_3\lambda(p) \tag{2.22}$$

on the momentum space $L^2(\mathbb{R}^2,\, dp)^2$.

Theorem 2.2. *The Dirac operator (2.12) is essentially self-adjoint on the dense domain* $\mathcal{S}(\mathbb{R}^2)^2$ [3] *and self-adjoint on the Sobolev space*

$$\mathrm{Dom}(\mathcal{D}) = H^1(\mathbb{R}^2)^2 = \left\{\psi \in L^2(\mathbb{R}^2,\, dx)^2 | \left(1+|p|^2\right)^{\frac{1}{2}}(\mathcal{F}\psi) \in L^2(\mathbb{R}^2,\, dp)^2\right\}. \tag{2.23}$$

Its spectrum is purely absolutely continuous and given by

$$\sigma(\mathcal{D}) = (-\infty, -m] \cup [m, +\infty). \tag{2.24}$$

Proof. We know from (2.22) that the Dirac operator $\mathcal{D}$ is unitarily equivalent to $\sigma_3\lambda(\cdot)$, and then it is self-adjoint on

$$\mathrm{Dom}(\mathcal{D}) = \mathcal{W}^{-1}\,\mathrm{Dom}(\sigma_3\lambda(\cdot)) = \mathcal{F}^{-1}u^{-1}\,\mathrm{Dom}(\lambda(\cdot)) = \mathcal{F}^{-1}\,\mathrm{Dom}(\lambda(\cdot)), \tag{2.25}$$

where we have used the fact that the multiplication by the unitary matrix $u^{-1}(p)$ does not modify the domain of any multiplication operator. By the very definition of $H^1(\mathbb{R}^2)^2$,

[2] In the Hilbert space $\mathcal{W}L^2(\mathbb{R}^2,\, dx)^2$ upper (lower) component spinors correspond to positive (negative) energies. Moreover, it is immediate to see that via the transformation $U_{FW} := \mathcal{F}^{-1}\mathcal{W}$, also knwon as *Foldy-Wouthuysen transformation* [118], the Dirac operator is unitarily equivalent to a pair of square-root Klein-Gordon equations

$$U_{FW}\mathcal{D}U_{FW}^{-1} = \begin{pmatrix} \sqrt{-\Delta+m^2} & 0 \\ 0 & -\sqrt{-\Delta+m^2} \end{pmatrix} \tag{2.21}$$

[3] This symbol denotes *Scwartz class functions*, that is, functions of rapid decrease [103].

it is the inverse Fourier transform of the set

$$\left\{\phi \in L^2(\mathbb{R}^2,\, dp)^2 |\, \left(1+|p|^2\right)^{\frac{1}{2}} \phi \in L^2(\mathbb{R}^2,\, dp)^2\right\}.$$

Then this set coincides with $\mathrm{Dom}(\lambda(\cdot))$. We thus conclude that the spectrum of $\mathcal{D}$ equals the spectrum of the multiplication operator $\sigma_3\lambda$ on the momentum space, which is simply given by the range of the functions $\lambda_i(p), i = 1{,}2$.

Consider the Dirac operator on the domain $\mathcal{S}(\mathbb{R}^2)^2$, and denote it by $\tilde{\mathcal{D}}$

$$\mathrm{Dom}(\tilde{\mathcal{D}}) = \mathcal{S}(\mathbb{R}^2)^2, \qquad \tilde{\mathcal{D}}\psi = -i\boldsymbol{\sigma}\cdot\nabla\psi + m\psi, \psi \in \mathcal{S}(\mathbb{R}^2)^2. \tag{2.26}$$

Recall that $\mathcal{S}(\mathbb{R}^2)^2$ is invariant with respect to the Fourier transform, and then $\tilde{\mathcal{D}}$ is unitarily equivalent to the restriction of the multiplication operator $h(p)$ to $\mathcal{S}(\mathbb{R}^2)^2$. The latter is essentially self-adjoint, as its closure is the self-adjoint operator $h(p)$, and the same holds for $\tilde{\mathcal{D}}$ and its closure is $\mathcal{D}$, the self-adjoint Dirac operator.

The fact that

$$\sigma(\mathcal{D}) = \sigma_{ac}(\mathcal{D}) = (-\infty, m] \cup [m, +\infty)$$

follows from (2.15),(2.16). See also [103, Ch. VII] □

2.2 Local boundary conditions on a bounded domain $\Omega \subset \mathbb{R}^2$

As explained in Section 1.1, the hexagonal symmetry implies that in absence of external fields low-energy electronic excitations behave as massless Dirac fermions. Rather than using the effective hamiltonian (1.12), it is more convenient to work in the so-called *isotropic representation* [9] and then to consider the hamiltonian

$$H = v_F \mathbb{1} \otimes (\boldsymbol{\sigma}\cdot(i\nabla)) = \begin{pmatrix} \mathcal{D} & 0 \\ 0 & \mathcal{D} \end{pmatrix}, \qquad \text{on} \quad L^2(\mathbb{R}^2, \mathbb{C}^2) \oplus L^2(\mathbb{R}^2, \mathbb{C}^2). \tag{2.27}$$

One can check that

$$H = UH_0U^{-1}, \qquad U = \frac{1}{2}\left(\mathbb{1}+\sigma_3\right)\otimes\mathbb{1} + \frac{1}{2}\left(\mathbb{1}-\sigma_3\right)\otimes\sigma_3, \tag{2.28}$$

and then the hamiltonians H_0 and H are unitarily equivalent, through the transformation U. The form of the operator H takes into account the fact that there are two inequivalent Dirac points (or valleys) $\boldsymbol{K}$ and $\boldsymbol{K}'$ in the first Brillouin zone of the honeycomb lattice. In the case where the contributions from the two Dirac points do not couple, it is sufficient to study the operator $\mathcal{D}$.

Consider a bounded domain $\Omega \subset \mathbb{R}^2$, which corresponds to a region of the plane where the (quasi-)particles are confined. Then one should impose boundary conditions for $\mathcal{D}$, which may break the block-diagonal structure in (2.27). That choice may change the spectrum of the resulting operator and thus the transport properties of graphene ribbons [9, 90]. Particularly important for practical purposes is the presence of a gap around zero, which turns graphene into a semiconductor. In this section we shall quickly recall the definition and basic properties of a family of boundary conditions for the Dirac operator which includes zigzag, armchair and infinite mass boundary conditions, following the recent works [19, 20].

Dealing with a bounded domain, one has to find necessary conditions that make the Dirac operator $\mathcal{D}$ symmetric on Ω. Let $u, v \in H^1(\Omega, \mathbb{C}^2)$, then integration by parts and the hermiticity of Pauli matrices imply that

$$\begin{aligned}\langle u, \mathcal{D}v\rangle_{L^2} &= \int_{\mathcal{D}} -i(u, \boldsymbol{\sigma}\cdot\nabla v)_{\mathbb{C}^2} = \int_{\mathcal{D}} -i\nabla\cdot(u, \boldsymbol{\sigma} v)_{\mathbb{C}^2} + i\int_{\Omega}(\boldsymbol{\sigma}\cdot\nabla u, v)_{\mathbb{C}^2} \\ &= \langle \mathcal{D}u, v\rangle_{L^2} - i\int_{\partial\Omega}(u, \boldsymbol{n}\cdot\boldsymbol{\sigma} v)_{\mathbb{C}^2},\end{aligned} \tag{2.29}$$

where $\boldsymbol{n}$ is the outward vector to $\partial\Omega$. Then the boundary term in (2.29) must vanish.

Consider the orthogonal projectors $\mathrm{P}_{\pm,\eta}$ defined as

$$\mathrm{P}_{\pm,\eta} = \frac{1}{2}(\mathbb{1}_2 \pm \mathrm{A}_\eta), \qquad \mathrm{A}_\eta = \cos(\eta)\boldsymbol{\sigma}\cdot\boldsymbol{t} + \sin(\eta)\sigma_3, \tag{2.30}$$

$\boldsymbol{t}$ being the unit vector tangent to the boundary $\partial\Omega$ and $\eta : \partial\Omega \longrightarrow \mathbb{R}$. Define

$$\mathrm{Dom}(\mathcal{D}_\eta) := \left\{u \in H^1(\Omega, \mathbb{C}^2) | (\mathrm{P}_{\text{-},\eta}\circ\gamma)u = 0\right\}, \tag{2.31}$$

where γ is the trace operator on $\partial\Omega$. Here we denote by the operator acting as $\mathcal{D}$ and with domain (2.31). The anticommutation relations of Pauli matrices give

$$\{\mathrm{A}_\eta, \boldsymbol{n}\cdot\boldsymbol{\sigma}\} = 0. \tag{2.32}$$

A direct calculation shows that the boundary term in (2.29) cancels and the operator $\mathcal{D}_\eta$ is symmetric.

Remark 2.3. Recall that for any $\phi \in \mathrm{Dom}(\mathcal{D}_\eta)$,

$$J_\phi(x) = (\phi(x), \boldsymbol{\sigma}\phi(x))_{\mathbb{C}^2} \tag{2.33}$$

can be interpreted as the current density [9, 113]. Then, as shown in [9], the condition

(2.32) is equivalent to the vanishing of the normal component of the current density in the state ϕ

$$(\phi, \boldsymbol{n} \cdot \boldsymbol{\sigma}\phi)_{\mathbb{C}^2} = 0, \tag{2.34}$$

that is, there is no current normal to the boundary of Ω and thus quasi-particles are confined in Ω.

The self-adjointness of $\mathcal{D}_\eta$ can be proved in the case of C^∞ boundaries adapting the results of [25] to the present case. However, a simpler proof which works at limited regularity has been recently given in [19], where the following theorem has been proved.

Theorem 2.4. *Given a bounded domain $\Omega \subset \mathbb{R}^2$ with C^2 boundary, and $\eta \in C^1(\partial\Omega)$, consider $\mathcal{D}_\eta$ as above. Then if $\cos(\eta(s)) \neq 0$, for all $s \in \partial\Omega$, the operator $\mathcal{D}_\eta$ is self-adjoint on $\mathrm{Dom}(\mathcal{D}_\eta)$. Moreover the spectrum $\sigma(\mathcal{D}_\eta) \subseteq \mathbb{R}$ of $\mathcal{D}_\eta$ is purely discrete and accumulates at $\pm\infty$.*

Remark 2.5. A priori the function η could be arbitrary, but in most physically relevant cases it is constant on the connected components of the boundary $\partial\Omega$, as explained in the following.

Remark 2.6. The spectrum of $\mathcal{D}_\eta$ is discrete as a consequence of the compactness of the Sobolev embedding $H^1(\Omega) \hookrightarrow L^2(\Omega)$.

For constant η and simply connected domains Ω the following lower bound for the spectral gap are proved in [20].

Theorem 2.7. *Take $\Omega \subset \mathbb{R}^2$ be a simply connected domain with C^2-boundary and let η be a constant such that $\cos\eta \neq 0$ and define $\mathcal{D}_\eta$ as above. Define $B = \min\left(\left|\frac{\cos\eta}{1-\sin\eta}\right|, \left|\frac{1-\sin\eta}{\cos\eta}\right|\right)$. If $\lambda \in \sigma(\mathcal{D}_\eta)$, then*

$$\lambda^2 \geqslant \frac{2\pi}{|\Omega|} B. \tag{2.35}$$

Following [20], we quickly explain how zigzag, infinite mass and armchair boundary conditions can be described in the above framework, working with the full operator (2.27). We adopt the notations of [9]. We shall consider uniform boundary conditions (η is constant) and then we will drop the dependence on η. Then boundary conditions for H, fulfilled by four-spinors are of the form

$$\mathrm{P}_-(A)\psi := \frac{1}{2}\left(\mathbb{1}_4 - A\right)\psi = 0 \qquad \text{on} \quad \partial\Omega, \tag{2.36}$$

where A is a 4×4 unitary matrix belonging to family of matrices explicitly computed in [9], see Section 1.2.3.

Zigzag boundary conditions. These conditions do not mix the valleys, and the matrix A is the following block matrix

$$A = \begin{pmatrix} \sigma_3 & \mathbb{0}_2 \\ \mathbb{0}_2 & -\sigma_3 \end{pmatrix}. \tag{2.37}$$

This matrix corresponds to the choice $\eta \equiv \frac{\pi}{2}$, and then to two copies of $\mathcal{D}_{\frac{\pi}{2}}$. Remark that this case is not covered by Theorem 2.4. It has been proved in [108], *ante litteram*, that the zigzag Dirac operator $\mathcal{D}_{\frac{\pi}{2}}$ is not self-adjoint on $H^1(\Omega, \mathbb{C}^2)$ as it has zero as an eigenvalue of infinite multiplicity. Then its domain cannot be included in $H^1(\Omega, \mathbb{C}^2)$ (see Remark 2.6). It has been described in [108].

Infinite mass boundary conditions. The matrix encoding the boundary conditions in this case is

$$A = \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{t} & \mathbb{0}_2 \\ \mathbb{0}_2 & -\boldsymbol{\sigma} \cdot \boldsymbol{t} \end{pmatrix} \tag{2.38}$$

and does not mix the valleys. We get a block-diagonal operator $\mathcal{D}_0 \oplus \mathcal{D}_\pi$ and Theorem 2.4 applies. Here the domain is $\mathrm{Dom}(\mathcal{D}_0) \oplus \mathrm{Dom}(\mathcal{D}_\pi) \subseteq H^1(\Omega, \mathbb{C}^4)$.

Armchair boundary conditions. The boundary conditions are given by

$$A = \begin{pmatrix} \mathbb{0}_2 & \nu^* \boldsymbol{\sigma} \cdot \boldsymbol{t} \\ \nu \boldsymbol{\sigma} \cdot \boldsymbol{t} & \mathbb{0}_2 \end{pmatrix} \tag{2.39}$$

with $|\nu| = 1$. These boundary conditions can be put into a block-diagonal form as follows. Using the unitary transformation

$$U_\nu = \begin{pmatrix} \nu \mathbb{1}_2 & \mathbb{0}_2 \\ \mathbb{0}_2 & \mathbb{1}_2 \end{pmatrix}, \tag{2.40}$$

one can, without loss of generality, consider only the case $\nu = 1$. We can act on the matrix A via the unitary transformation

$$V = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \tag{2.41}$$

which exchanges the second and fourth spinor components. This converts the boundary conditions into

$$B = VAV^* = \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{t} & \mathbb{0}_2 \\ \mathbb{0}_2 & \boldsymbol{\sigma} \cdot \boldsymbol{t} \end{pmatrix}, \tag{2.42}$$

and transforms the Hamiltonian as

$$K = VHV^* = \begin{pmatrix} \mathbb{0}_2 & \mathcal{D} \\ \mathcal{D} & \mathbb{0}_2 \end{pmatrix}. \tag{2.43}$$

Then also the armchair boundary conditions can be included in this description.

In the following (see Chapter 4) we will be particularly interested in infinite mass boundary conditions. In this case $\eta \equiv 0$ or $\eta \equiv \pi$ and then $\mathrm{A}_\eta = \pm \boldsymbol{\sigma} \cdot \boldsymbol{t}$. Then using the anticommutation properties of Pauli matrices, a direct calculation shows that the domain of the operator $\mathrm{Dom}(\mathcal{D}_{0,\pi})$ is invariant with respect to the antiunitary transformation $\mathcal{U} := \sigma_1 \mathcal{C}$, where $\mathcal{C}$ is the complex conjugation on $L^2(\Omega, \mathbb{C}^2)$. Given $\varphi \in \mathrm{Dom}(\mathcal{D}_{0,\pi})$ we have

$$\mathcal{U}\mathcal{D}_{0,\pi}\varphi = -\mathcal{D}_{0,\pi}\mathcal{U}\varphi.$$

Moreover, in this case the constant B appearing in the gap estimates (2.7) is equal to 1. We summarize the above observations in the following

Proposition 2.8. *The spectrum of the Dirac operator with infinite mass boundary conditions $\mathcal{D}_{0,\pi}$ is discrete, symmetric and accumulates to $\pm\infty$. Moreover, if λ is an eigenvalue of $\mathcal{D}_{0,\pi}$ there holds*

$$\lambda^2 \geqslant \frac{2\pi}{|\Omega|}. \tag{2.44}$$

We remark that in [113], Stockmeyer and Vugalter proved that infinite mass Dirac operators are the limit, in a suitable sense, of Dirac operators on $\mathbb{R}^2$ with a mass term supported outside Ω. More precisely, given $M > 0$ define the following Dirac operator with domain $H^1(\mathbb{R}^2, \mathbb{C}^2)$

$$H_M = \mathcal{D} + \sigma_3 M(1 - \chi_\Omega), \tag{2.45}$$

where χ_Ω denotes the characteristic function of Ω. Since the domain Ω is bounded, it is easy to see that the operator H_M is a compact perturbation of the self-adjoint operator $\mathcal{D}_M$ and then $\sigma_{ess}(H_M) = \sigma_{ess}(\mathcal{D}_M)$ (see the previous section) and it has purely discrete spectrum on $(-M, M)$ (see [103, Thm S.13]). Let us denote the infinite mass Dirac operator by H_∞. The main result proven in [113] is the following

Theorem 2.9. *(Convergence of spectral projections) Let Ω be a connected bonded domain with C^3 boundary and let λ be an eigenvalue of H_∞. Then for any $0 < \varepsilon < \mathrm{dist}(\sigma(H_\infty))$, there holds*

$$\left\| \tilde{E}_{\{\lambda\}}(H_\infty) - E_{(\lambda-\varepsilon,\lambda+\varepsilon)}(H_M) \right\| \longrightarrow 0 \qquad \text{as} \quad M \longrightarrow +\infty, \tag{2.46}$$

where we have rewritten the spectral projector $\tilde{E}_{\{\lambda\}}(H_\infty) = E_{\{\lambda\}}(H_\infty) \oplus \{0\}$ in terms of the splitting

$$L^2(\mathbb{R}^2, \mathbb{C}^2) = L^2(\Omega, \mathbb{C}^2) \oplus L^2(\mathbb{R}^2 \setminus \Omega, \mathbb{C}^2).$$

In particular, the eigenvalues of H_M converge toward those of H_∞ as $M \to +\infty$ and any eigenvalue of H_∞ is the limit of eigenvalues of H_M.

The above result justifies, in some sense, the name ”infinite mass” adopted for those boundary conditions.

2.3 Quantum graphs with Kirchoff-type conditions

The aim of this section is to present some basics on metric graphs and on the Dirac operator, needed for the results contained in Chapter 5. This is part of a joint work with Raffaele Carlone and Lorenzo Tentarelli [29].

2.3.1 Metric graphs and functional setting

A complete discussion of the definition and the features of metric graphs can be found in [3, 21, 78] and the references therein. Here we limit ourselves to recall some basic notions.

Throughout, a *metric graph* $\mathcal{G} = (\mathrm{V}, \mathrm{E})$ is a connected *multigraph* (i.e., multiple edges and self-loops are allowed) with a finite number of edges and vertices. Each edge is a finite or half-infinite segment of line and the edges are glued together at their endpoints (the vertices of $\mathcal{G}$) according to the topology of the graph (see Figure 5.1).

Unbounded edges are identified with (copies of) $\mathbb{R}^+ = [0, +\infty)$ and are called half-lines, while bounded edges are identified with closed and bounded intervals $I_e = [0, \ell_e]$, $\ell_e > 0$. Each edge (bounded or unbounded) is endowed with a coordinate x_e, chosen in the corresponding interval, which has an arbitrary orientation if the interval is bounded, whereas presents the natural orientation in case of a half-line.

As a consequence, the graph $\mathcal{G}$ is a locally compact metric space, the metric given by the shortest distance along the edges. Clearly, since we assume a finite number of edges and vertices, $\mathcal{G}$ is *compact* if and only if it does not contain any half-line. A further important notion, introduced in [4, 111] is the following.

Definition. If $\mathcal{G}$ is a metric graph, we define its *compact core* $\mathcal{K}$ as the metric subgraph of $\mathcal{G}$ consisting of all its bounded edges. In addition, we denote by ℓ the measure of $\mathcal{K}$, namely

$$\ell = \sum_{e\in\mathcal{K}} \ell_e.$$

A function $u : \mathcal{G} \to \mathbb{C}$ can be regarded as a family of functions (u_e), where $u_e : I_e \to \mathbb{C}$ is the restriction of u to the edge (represented by) I_e. The usual L^p spaces can be defined in the natural way, with norm

$$\|u\|^p_{L^p(\mathcal{G})} := \sum_{e\in\mathrm{E}} \|u_e\|^p_{L^p(I_e)}, \quad \text{if } p \in [1, \infty), \qquad \text{and} \qquad \|u\|_{L^\infty(\mathcal{G})} := \max_{e\in\mathrm{E}} \|u_e\|_{L^\infty(I_e)},$$

while $H^1(\mathcal{G})$ is the space of functions $u = (u_e)$ such that $u_e \in H^1(I_e)$ for every edge $e \in \mathrm{E}$, with norm

$$\|u\|^2_{H^1(\mathcal{G})} = \|u'\|^2_{L^2(\mathcal{G})} + \|u\|^2_{L^2(\mathcal{G})}$$

(and in this way one can also define $H^2(\mathcal{G})$, $H^3(\mathcal{G})$, etc ...). Consistently, a spinor $\psi = (\psi^1, \psi^2)^T : \mathcal{G} \to \mathbb{C}^2$ is a family of 1d-spinors

$$\psi_e = \begin{pmatrix} \psi^1_e \\ \psi^2_e \end{pmatrix} : I_e \longrightarrow \mathbb{C}^2, \qquad \forall e \in \mathrm{E},$$

and thus

$$L^p(\mathcal{G}, \mathbb{C}^2) := \bigoplus_{e\in\mathrm{E}} L^p(I_e) \otimes \mathbb{C}^2,$$

endowed with the norm

$$\|\psi\|^p_{L^p(\mathcal{G},\mathbb{C}^2)} := \sum_{e\in\mathrm{E}} \|\psi_e\|^p_{L^p(I_e)}, \quad \text{if } p \in [1, \infty), \qquad \text{and} \qquad \|\psi\|_{L^\infty(\mathcal{G},\mathbb{C}^2)} := \max_{e\in\mathrm{E}} \|\psi_e\|_{L^\infty(I_e)},$$

while

$$H^1(\mathcal{G}, \mathbb{C}^2) := \bigoplus_{e\in\mathrm{E}} H^1(I_e) \otimes \mathbb{C}^2$$

endowed with the norm

$$\|\psi\|^2_{H^1(\mathcal{G},\mathbb{C}^2)} := \sum_{e\in\mathrm{E}} \|\psi_e\|^2_{H^1(I_e)}$$

(and so on for $H^2(\mathcal{G}, \mathbb{C}^2)$, $H^3(\mathcal{G}, \mathbb{C}^2)$, etc ...). Equivalently, one can say that $L^p(\mathcal{G}, \mathbb{C}^2)$ is the space of the spinors such that $\psi^1, \psi^2 \in L^p(\mathcal{G})$, with

$$\|\psi\|^p_{L^p(\mathcal{G},\mathbb{C}^2)} := \|\psi^1\|^p_{L^p(\mathcal{G})} + \|\psi^2\|^p_{L^p(\mathcal{G})}, \quad \text{if } p \in [1,\infty),$$

$$\|\psi\|_{L^\infty(\mathcal{G},\mathbb{C}^2)} := \max\left\{\|\psi^1\|_{L^\infty(\mathcal{G})}, \|\psi^2\|_{L^\infty(\mathcal{G})}\right\},$$

and that $H^1(\mathcal{G},\mathbb{C}^2)$ is the space of the spinors such that $\psi^1, \psi^2 \in H^1(\mathcal{G})$, with

$$\|\psi\|^2_{H^1(\mathcal{G},\mathbb{C}^2)} := \|\psi^1\|^2_{H^1(\mathcal{G})} + \|\psi^2\|^2_{H^1(\mathcal{G})}.$$

Remark 2.10. In the literature on metric graphs, the usual definition of the space $H^1(\mathcal{G})$ consists also of a global continuity requirement, which forces all the components of a function that are incident to a vertex to assume the same value at that vertex. However, in this case it is worth keeping this global continuity notion separate and introduce it when it is actually required (see (5.16)).

Remark 2.11. In view of the isomorphism $L^p(\mathcal{G},\mathbb{C}^2) \simeq L^p(\mathcal{G}) \otimes \mathbb{C}^2, 1 \leqslant p \leqslant \infty$ we will interchangeably use both notations, and similarly for other spaces of vector valued functions. A similar notation will be correspondingly adopted also for differential operators.

2.3.2 The Dirac operator with Kirchhoff-type conditions

We want to study the spectral properties of the following Dirac operator on the graph $\mathcal{G}$

$$\mathcal{D} := -\imath c \frac{d}{dx} \otimes \sigma_1 + mc^2 \otimes \sigma_3, \tag{2.47}$$

The expression given by (2.47) of the Dirac operator is purely formal, since it does not clarify what happens at the vertices of the graph, given that the derivative $\frac{d}{dx}$ is well defined just in the interior of the edges.

As well as for the laplacian in the Schrödinger case, the way to give a rigorous meaning to (2.47) is to find suitable self-adjoint realizations of the operator imposing suitable vertex conditions. However, an extensive discussion of all the possible self-adjoint realizations of the Dirac operator on graphs goes beyond the aims of this thesis. We limit ourselves to the case of the Kirchhoff-type conditions (introduced in [106]) which represent the free case for the Dirac operator, namely, the case in which there are no attractive or repulsive effects at the vertices, which then play the role of mere junctions between the edges. Roughly speaking these conditions "split" the requirements of Kirchhoff conditions: the continuity condition is imposed only on the first component of the spinor, while the second component (in place of the derivative) has to satisfy a "balance" condition (see (2.49)&(2.50)).

For more details on self-adjoint extensions of the Dirac operator on metric graphs we refer the reader to [101, 33].

Definition. Let $\mathcal{G}$ be a metric graph and let $m, c > 0$. We call *Dirac operator* with Kirchhoff-type boundary conditions the operator $\mathcal{D} : L^2(\mathcal{G}, \mathbb{C}^2) \to L^2(\mathcal{G}, \mathbb{C}^2)$ with action

$$\mathcal{D}_{|_{I_e}}\psi = \mathcal{D}_e\psi_e := -\imath c\,\sigma_1\psi_e' + mc^2\,\sigma_3\psi_e, \qquad \forall e \in \mathrm{E},$$

σ_1, σ_3 being the matrices defined in (5.4), and domain

$$\mathrm{dom}(\mathcal{D}) := \left\{\psi \in H^1(\mathcal{G}, \mathbb{C}^2) : \psi \text{ satisfies (2.49) and (2.50)}\right\}, \tag{2.48}$$

where

$$\psi_e^1(\mathrm{v}) = \psi_f^1(\mathrm{v}), \qquad \forall e, f \succ \mathrm{v}, \qquad \forall \mathrm{v} \in \mathcal{K}, \tag{2.49}$$

$$\sum_{e \succ v} \psi_e^2(\mathrm{v})_\pm = 0, \qquad \forall \mathrm{v} \in \mathcal{K}, \tag{2.50}$$

"$e \succ v$" meaning that the edge e is incident at the vertex v and $\psi_e^2(\mathrm{v})_\pm$ standing for $\psi_e^2(0)$ or $-\psi_e^2(\ell_e)$ according to whether x_e is equal to 0 or ℓ_e at v.

Remark 2.12. Note that the operator $\mathcal{D}$ actually depends of the parameters m, c, which represent the mass of the generic particle described by the operator and the speed of light (respectively). For the sake of simplicity we omit this dependence unless it be necessary to avoid misunderstandings.

The basic properties of the operator (2.47) with the above conditions are summarized in the following

Proposition. *The Dirac operator* (2.47) *with Kirchoff-type conditions* (2.49),(2.50) *is self-adjoint on* $L^2(\mathcal{G}, \mathbb{C}^2)$ *with domain* (2.48). *Moreover its spectrum is given by*

$$\sigma(\mathcal{D}) = (-\infty, -mc^2] \cup [mc^2, +\infty). \tag{2.51}$$

Using well-known results from the literature about selfadjoint extensions one can prove that linear boundary conditions like (2.49), (2.50) lead to a selfadjoint Dirac operator on a graph (see, e.g. [33, 94, 10, 100]). In particular, the main result in [33] proves self-adjointness for Dirac operators on metric graphs with a wide family of linear vertex conditions, including the Kirchoff-type conditions (2.49),(2.50).

In order to study the spectral properties of the operator (2.47) one first has to study the operator on the single components of the graph (segments and halflines) imposing suitable boundary conditions. Then one needs to describe the effect of connecting those one-dimensional components according to the topology of the graph, through the vertex condtions (2.49),(2.50). This can be achieved, for instance, using the theory of *boundary triplets*. In this section we limit ourselves to a brief presentation of the main ideas and techniques. We refer the reader to [38, 62] and references therein for more details.

Preliminarly let us recall some basic notions. Let A be a densely defined closed symmetric operator in a separable Hilbert space $\mathcal{H}$ with equal deficiency indices $\mathrm{n}_\pm(A) = \dim \mathcal{N}_{\pm \mathrm{i}} \leqslant \infty$, where $\mathcal{N}_z := \ker(A^* - z)$ is the defect subspace.

Definition. A triplet $\Pi = \{\mathfrak{H}, \Gamma_0, \Gamma_1\}$ is called a boundary triplet for the adjoint operator A^* if $\mathfrak{H}$ is an auxiliary Hilbert space and $\Gamma_0, \Gamma_1 : \operatorname{dom}(A^*) \to \mathfrak{H}$ are linear mappings such that the second abstract Green identity

$$(A^* f, g) - (f, A^* g) = (\Gamma_1 f, \Gamma_0 g)_{\mathfrak{H}} - (\Gamma_0 f, \Gamma_1 g)_{\mathfrak{H}}, \qquad f, g \in \operatorname{dom}(A^*), \tag{2.52}$$

holds and the mapping $\Gamma := \begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix} : \operatorname{dom}(A^*) \to \mathfrak{H} \oplus \mathfrak{H}$ is surjective.

Let us consider $A_0 := A^* \restriction \ker \Gamma_0$ and its resolvent set $\rho(A_0)$.

The operator valued functions $\gamma(\cdot) : \rho(A_0) \to \mathcal{L}(\mathcal{H}, \mathfrak{H})$ and $M(\cdot) : \rho(A_0) \to \mathcal{L}(\mathcal{H})$ defined by

$$\gamma(z) := \left(\Gamma_0 \restriction \mathcal{N}_z\right)^{-1} \qquad \text{and} \qquad M(z) := \Gamma_1 \gamma(z), \qquad z \in \rho(A_0), \tag{2.53}$$

are called the *γ-field* and the *Weyl function*, respectively, corresponding to the boundary triplet Π.

The graph $\mathcal{G}$ can be decomposed in finite length edges $e \in \mathrm{E}_s$ identified with segments $I_e = [0, \ell_e]$, and non-compact edges E_h identified with half-lines $\mathbb{R}_+ = [0, +\infty)$.

Consider a finite edge $e \in \mathrm{E}_s$ of the graph and the corresponding minimal operator $\widetilde{D_e}$ on $\mathcal{H}_e = L^2(I_e) \otimes \mathbb{C}^2$ given by the differential expression

$$\mathcal{D} = -i\, c\, \frac{d}{dx} \otimes \sigma_1 + mc^2 \otimes \sigma_3 = \begin{pmatrix} mc^2 & -i\, c\, \frac{d}{dx} \\ -i\, c\, \frac{d}{dx} & -mc^2 \end{pmatrix}, \tag{2.54}$$

and with domain $H_0^1(I_e) \otimes \mathbb{C}^2$. The domain of the adjoint operator (formally acting as $\mathcal{D}$) is

$$\operatorname{Dom}(\widetilde{D_e^*}) = H^1(I_e) \otimes \mathbb{C}^2.$$

A suitable choice of trace operators [62] is $\Gamma^e_{0,1} : H^1(I_e) \otimes \mathbb{C}^2 \to \mathbb{C}^2$, defined by

$$\Gamma^e_0 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \psi_1(0) \\ ic\psi_1(\ell_e) \end{pmatrix}, \qquad \Gamma^e_1 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} ic\psi_2(0) \\ \psi_2(\ell_e) \end{pmatrix}. \tag{2.55}$$

Given the boundary triplet $\{\mathfrak{H}_e, \Gamma^e_0, \Gamma^e_1\}$, with $\mathfrak{H}_e = \mathbb{C}^2$, one can find the gamma field and the Weyl function, defined as in (2.53). Moreover, it can be proved that the above operator has defect indices $n_\pm(\widetilde{\mathcal{D}_e}) = 2$. Remark that the operator

$$\mathcal{D}_e = \widetilde{\mathcal{D}^*_e}, \qquad \mathrm{Dom}(\mathcal{D}_e) = \ker \Gamma^e_0, \tag{2.56}$$

is self-adjoint, *by construction*.

Analogously, for a half-line $e' \in \mathrm{E}_h$ we consider the minimal operator $\widetilde{\mathcal{D}_{e'}}$ given by the same differential expression (2.54) on $\mathcal{H}_{e'} = L^2(\mathbb{R}_+) \otimes \mathbb{C}^2$, with domain $H^1_0(\mathbb{R}_+) \otimes \mathbb{C}^2$. The adjoint operator has domain

$$\mathrm{Dom}(\widetilde{\mathcal{D}^*_{e'}}) = H^1(\mathbb{R}_+) \otimes \mathbb{C}^2.$$

In this case the trace operators $\Gamma^{e'}_{0,1} : H^1(\mathbb{R}_*) \otimes \mathbb{C}^2 \to \mathbb{C}$ can be defined as

$$\Gamma^{e'}_0 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \psi_1(0), \qquad \Gamma^{e'}_1 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = ic\psi_2(0), \tag{2.57}$$

and one can find the gamma field and the Weyl function, as for the case of the segment, with respect to the boundary triplet $\left\{\mathfrak{H}_{e'}, \Gamma^{e'}_0, \Gamma^{e'}_1\right\}$, with $\mathfrak{H}_{e'} = \mathbb{C}$. Moreover, one can show that the operator $\widetilde{\mathcal{D}_{e'}}$ has defect indices $n_\pm(\widetilde{\mathcal{D}_{e'}}) = 1$. As before, we can define a self-adjoint operator as a restriction of the adjoint, as

$$\mathcal{D}_{e'} = \widetilde{\mathcal{D}^*_{e'}}, \qquad \mathrm{Dom}(\mathcal{D}_{e'}) = \ker \Gamma^e_0. \tag{2.58}$$

Consider the following operator on $\mathcal{H} = \bigoplus_{e \in \mathrm{E}_s} \mathcal{H}_e \oplus \bigoplus_{e' \in \mathrm{E}_h} \mathcal{H}_{e'}$ defined as the direct sum

$$\mathcal{D}_0 := \bigoplus_{e \in \mathrm{E}_s} \mathcal{D}_e \oplus \bigoplus_{e' \in \mathrm{E}_h} \mathcal{D}_{e'}, \tag{2.59}$$

whose domain is given by the direct sum of the domains of the summands. The spectrum of the operator $\mathcal{D}_0$, it is given by the superposition of the spectra of each summand, that is

$$\sigma(\mathcal{D}_0) = \bigcup_{e\in \mathrm{E}_s} \sigma(\mathcal{D}_e) \cup \bigcup_{e'\in \mathrm{E}_h} \sigma(\mathcal{D}_{e'}) \tag{2.60}$$

Precisely, in [38] it is proved that each segment I_e, $e \in \mathrm{E}_s$ contributes to the point spectrum of $\mathcal{D}_0$ with eigenvalues given by

$$\sigma(\mathcal{D}_e) = \sigma_p(\mathcal{D}_e) = \left\{ \pm\sqrt{\frac{2mc^2\pi^2}{\ell_e^2}\left(j+\frac{1}{2}\right)^2 + m^2c^4}\ ,\ j\in\mathbb{N} \right\}, \qquad \forall e \in \mathrm{E}_s, \tag{2.61}$$

while the spectrum on half-lines, on the contrary, is purely absolutely continuous and is given by

$$\sigma(\mathcal{D}_e) = \sigma_{ac}(\mathcal{D}_e) = (-\infty, -mc^2] \cup [mc^2, +\infty), \qquad \forall e \in \mathrm{E}_h. \tag{2.62}$$

Let us now describe the Dirac operator with vertex conditions (2.49),(2.50) using the boundary triplets formalism. Consider the operator

$$\widetilde{\mathcal{D}} := \bigoplus_{e\in \mathrm{E}_s} \widetilde{\mathcal{D}_e} \oplus \bigoplus_{e'\in \mathrm{E}_h} \widetilde{\mathcal{D}_{e'}}, \tag{2.63}$$

and its adjoint

$$\widetilde{\mathcal{D}^*} := \bigoplus_{e\in \mathrm{E}_s} \widetilde{\mathcal{D}_e^*} \oplus \bigoplus_{e'\in \mathrm{E}_h} \widetilde{\mathcal{D}_{e'}^*}, \tag{2.64}$$

with obvious definition of the domains. Define the trace operators

$$\Gamma_{0,1} = \bigoplus_{e\in \mathrm{E}_s} \Gamma_{0,1}^e \oplus \bigoplus_{e'\in \mathrm{E}_h} \Gamma_{0,1}^{e'}.$$

One can prove that $\{\mathfrak{H}, \Gamma_0, \Gamma_1\}$, with $\mathfrak{H} = \mathbb{C}^M$ and $M = 2|\mathrm{E}_s| + |\mathrm{E}_h|$, is a boundary triplet for the operator $\widetilde{\mathcal{D}^*}$, and it is possible to find the corresponding gamma-field and Weyl function, as already remarked. Notice that boundary conditions (2.49),(2.50) are ”local”, in the sense that at each vertex they are expressed independently from the conditions on other vertices. As a consequence, they are expressed by suitable block diagonal matrices $A, B \in \mathbb{C}^{M\times M}$ with $AB^* = BA^*$. Then conditions (2.49),(2.50) can be written as

$$A\Gamma_0\psi = B\Gamma_1\psi. \tag{2.65}$$

The model case studied at the end of the section clarifies the above notation. Notice that the sign convention of (2.50) can be incorporated in the definition of the matrix B.

The Dirac operator with Kirchoff-type conditions is then defined as

$$\mathcal{D} = \widetilde{\mathcal{D}^*}, \qquad \mathrm{Dom}(\mathcal{D}) = \ker(A\Gamma_0 - B\Gamma_1), \tag{2.66}$$

and thus *by construction* the operator is self-adjoint.

Remark 2.13. The boundary triplets method provides an alternative way to prove the self-adjointness of the Dirac operator with conditions (2.49),(2.50), different from the classical approach *à la* Von Neumann adopted in [33]. However, in some sense those methods are equivalent.

As for the Schrödinger case [77], the following Krein-type formula for resolvent operators can be proved

$$(\mathcal{D} - z)^{-1} - (\mathcal{D}_0 - z)^{-1} = \gamma_z \left(B\, M(z) - A\right)^{-1} B\gamma_{\bar{z}}^*, \qquad \forall z \in \rho(\mathcal{D}) \cap \rho(\mathcal{D}_0), \tag{2.67}$$

and thus the resolvent of the operator $\mathcal{D}$ can be regarded as a perturbation of the resolvent of the operator $\mathcal{D}_0$. In the above formula γ_z and $M(z)$ are, respectively, the gamma-field and the Weyl function associated with $\mathcal{D}$ (see [38]). It turns out that the operator appearing in the right-hand side of (2.67) is of finite rank. As explained in [77] for the case of the laplacian, this is a consequence of the fact that each summand in (2.54) has finite defect indices (see again [38]).

Therefore using Weyl's Theorem [104, Thm XIII.14] one can conclude from (2.67) that

$$\sigma_{ess}(\mathcal{D}) = \sigma_{ess}(\mathcal{D}_0) = (-\infty, -mc^2] \cup [mc^2, +\infty). \tag{2.68}$$

Notice that the point eigenvalues (2.61) for $\mathcal{D}_0$ are embedded in the continuous spectrum (2.62). Then it remains to prove that they cannot enter the gap $(-m, m)$ as vertex conditions (2.49), (2.50) are imposed.

Let $\lambda \in \sigma(\mathcal{D})$ be an eigenvalue. Then for some $\psi \in \mathrm{Dom}(\mathcal{D})$, there holds

$$\mathcal{D}\psi = \lambda\psi. \tag{2.69}$$

In matrix notation the above equation reads as

$$\begin{pmatrix} mc^2 & -ic\frac{d}{dx} \\ -ic\frac{d}{dx} & -mc^2 \end{pmatrix} \begin{pmatrix} \psi^1 \\ \psi^2 \end{pmatrix} = \lambda \begin{pmatrix} \psi^1 \\ \psi^2 \end{pmatrix} \tag{2.70}$$

that is

$$
\begin{aligned}
-ic\frac{d\psi^2}{dx} &= (\lambda - mc^2)\psi^1,\\
-ic\frac{d\psi^1}{dx} &= (\lambda + mc^2)\psi^2.
\end{aligned}
\tag{2.71}
$$

Assuming $|\lambda| \neq m$, we can divide both sides of the second equation in (2.71) by $(\lambda + mc^2)$ and plug the value of ψ^2 into the other equation obtaining:

$$
-c^2\frac{d^2\psi^1}{dx^2} = (\lambda^2 - m^2c^4)\psi^1, \qquad \text{on} \quad \mathcal{G}. \tag{2.72}
$$

In addition, combining conditions (2.49),(2.50) give:

$$
\begin{aligned}
&\sum_{e\succ v}\frac{d\psi_e^1}{dx}(v)_{\pm} = 0,\\
&\psi_{e_i}^1(v) = \psi_{e_j}^1(v), \quad \forall e_i, e_j \succ v.
\end{aligned}
\tag{2.73}
$$

Then ψ^1 turns out to be an eigenfunction of the laplacian on $\mathcal{G}$, satisfying continuity and Kirchoff vertex conditions. Multiplying (2.72) by ψ^1 and integrating one concludes that

$$
|\lambda| > mc^2, \tag{2.74}
$$

thus proving that there are no eigenvalues of $\mathcal{D}$ in $(-mc^2, mc^2)$ for our choice of boundary conditions. Then we conclude that imposing the Kirchoff-type conditions the eigenvalues (2.61) can at most move to the tresholds $\pm mc^2$ but not enter the gap.

Remark 2.14. Singularities (eigenvalues, resonances...) of the resolvent correspond to the zeroes of $\det(B\,M(z) - A)$. However, a more detailed study of resonances formation is beyond the scope of the present work and will be the object of future investigation.

Let us consider, finally, an example to clarify the main idea of the definition of Kirchoff-type conditions in the above construction. The graph considered is a 3-star graph with a finite edge, as depicted in Figure 2.1.

In this case the finite edge is identified with the interval $I = [0, L]$ and 0 corresponds to the common vertex of the segment and the half-lines.

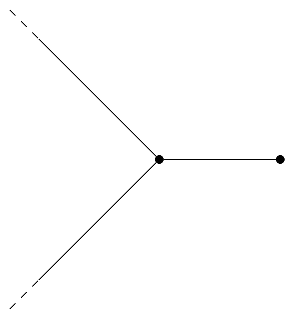

Figure 2.1. A 3-star graph with a finite edge.

Consider the trace operators

$$\Gamma_0\psi = \begin{pmatrix} \psi_1^{(1)}(0) \\ \psi_2^{(1)}(0) \\ \psi_3^{(1)}(0) \\ ic\psi_3^{(1)}(L) \end{pmatrix}, \quad \Gamma_1\psi = \begin{pmatrix} ic\psi_1^{(2)}(0) \\ ic\psi_2^{(2)}(0) \\ ic\psi_3^{(2)}(0) \\ \psi_3^{(2)}(L) \end{pmatrix}, \tag{2.75}$$

where ψ_k^j is the k-th component of the spinor on the j-th edge. Moreover, $k = 1{,}2$ correspond to the halflines, while $k = 3$ represents the segment.

The Kirchoff-type conditions (2.49), (2.50) can be rewritten as $A\Gamma_0\psi = B\Gamma_1\psi, \quad AB^* = BA^*$, where

$$A = \frac{2}{3}\begin{pmatrix} -2 & 1 & 1 & 0 \\ 1 & -2 & 1 & 0 \\ 1 & 1 & -2 & 0 \\ 0 & 0 & 0 & a \end{pmatrix}, \quad B = -\imath\frac{2}{3}\begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & b \end{pmatrix} \tag{2.76}$$

Choosing the parameters $a, b \in \mathbb{C}$ we can fix the value of the spinor on the non-connected vertex. Since, as already remarked, conditions (2.49), (2.50) are defined independently on each vertex, one can iterate the above construction for a more general graph structure. Then matrices A, B will have a block structure, each block corresponding to a vertex. For the sake of brevity we omit the details, as the idea of the construction is now clear.

Chapter 3

Cubic Dirac equations with Kerr nonlinearities in 2D

3.1 Introduction

The following nonlinear Schrödinger/Gross-Pitaevskii (NLS/GP) equation.

$$i\partial_t u = -\Delta u + V(x)u + \kappa|u|^2 u, \qquad x \in \mathbb{R}^2, \kappa \in \mathbb{R}, \tag{3.1}$$

describes, in the quantum setting, the dynamics of Bose-Enstein condensates, and u is the wavefunction of the condensate [99, 49]. Here $V(x)$ models a magnetic trap and the nonlinear potential $\kappa|u|^2$ describes a mean-field interaction between particles. The parameter κ is the microscopic 2-body scattering length. Another important field of application of NLS/GP is nonlinear optics, namely in the description of electromagnetic interference of beams in photorefractive crystals [93]. In this case $V(x)$ is determined by the spatial variations of the background linear refractive index of the medium, while the nonlinear potential accounts for the fact that regions of higher electric field intensity have a higher refractive index (the so-called Kerr nonlinear effect). In this case $\kappa < 0$ represents the Kerr nonlinearity coefficient. In the latter situation, the variable $t \in \mathbb{R}$ denotes the distance along the direction of propagation and $x \in \mathbb{R}^2$ the transverse dimensions. In the above systems, honeycomb structures can be realized and tuned through suitable optical induction techniques based on laser or light beam interference [69]. They are encoded in the properties of the periodic potential $V(x)$.

We assume that the potential $V(x)$ admits Dirac points in its dispersion relations, in the sense of Def. 1.5. Then as for the linear case (see section 1.2), one expects the

Dirac equation to appear as effective equation describing the dynamics of initial data concentrated at a Dirac point K. Moreover, the effective equation should contain a cubic nonlinearity, corresponding to the cubic term in (3.1) modulated by some coefficients which depend on the potential V. This is actually the case, as formally first computed in [80] where the authors showed that assuming spectrally concentrated intial data for (3.1)

$$u_0^\varepsilon(x) = \sqrt{\varepsilon}(\alpha_{0,1}(\varepsilon x)\Phi_1(x) + \alpha_{0,2}(\varepsilon x)\Phi_2(x)), \qquad x \in \mathbb{R}^2, \varepsilon > 0, \tag{3.2}$$

and making the ansatz

$$u^\varepsilon(t,x) = e^{-i\mu_* t}\left(\sum_{j=1}^{2}\sqrt{\varepsilon}\psi_j(\varepsilon t, \varepsilon x)\Phi_j(x) + \eta^\varepsilon(t,x)\right), \tag{3.3}$$

by a calculation similar to the one done for the linear case [57] one finds the following Dirac system for the amplitudes ψ_j

$$\begin{cases} \partial_t\psi_1 + \overline{\lambda_\#}(\partial_{x_1} + i\partial_{x_2})\psi_2 = -i\kappa(2\beta_2|\psi_1|^2 + \beta_1|\psi_2|^2)\psi_1 \\ \partial_t\psi_2 + \lambda_\#(\partial_{x_1} - i\partial_{x_2})\psi_1 = -i\kappa(\beta_1|\psi_1|^2 + 2\beta_2|\psi_2|^2)\psi_2 \end{cases}, \tag{3.4}$$

where

$$\beta_2 := \int_Y |\Phi_1(x)|^2|\Phi_2(x)|^2 dx \leqslant \beta_1 := \int_Y |\Phi_1(x)|^4 dx = \int_Y |\Phi_2(x)|^4 dx. \tag{3.5}$$

Here $\lambda_\# \in \mathbb{C} \setminus \{0\}$ is the same constant as in Def. 1.5 (see [57],[56]).

A rigorous derivation has been recently given by Arbunich and Sparber in [16], where the system (3.4) is obtained by a multiscale expansion.

Remark 3.1. The modulating coefficients are scaled so that the nonlinearity and the Dirac dynamics enter on the same time-scale. The factor $\sqrt{\varepsilon}$ corresponds here to the critical scaling, in this sense.

Theorem 3.2. *(Dirac dynamics for NLS/GP, [16]) Take $T > 0$ and $S > s + 3$ with $s > 1$. Consider a solution $\psi \in C([0,T), H^S(\mathbb{R}^2))^2$ to (3.4). Then for any $T_* \in [0,T)$ and considering initial data (3.2), the solution $u \in C([0, T_*\varepsilon^{-1}), H^s(\mathbb{R}^2))$ to the NLS/GP equation*

$$i\partial_t u = -\Delta u + V(x)u + \kappa|u|^2 u, \qquad x \in \mathbb{R}^2, \kappa \in \mathbb{R}, \tag{3.6}$$

is of the form (3.3) and there holds

$$\sup_{0\leqslant t\leqslant T_*\varepsilon^{-1}} \|\eta^\varepsilon(t,x)\|_{H^s_x(\mathbb{R}^2)} \xrightarrow{\varepsilon\to 0} 0. \tag{3.7}$$

In [16] the system (3.4) is obtained using a multiscale expansion. More precisely, one looks for an approximate solution to (3.6) of the form

$$u^\varepsilon(t,x) \simeq_{\varepsilon\to 0} u^\varepsilon_N(t,x) := e^{-i\mu_* t/\varepsilon}\sqrt{\varepsilon}\sum_{k=1}^{N}\varepsilon^k u_k(\varepsilon t,\varepsilon x,x), \qquad N\in\mathbb{N}. \tag{3.8}$$

Plugging the ansatz (3.8) into (3.6) formal computations show that the leading order term in the expansion is a modulation of Bloch functions, as in (3.3), where $\psi = (\psi_1,\psi_2)^T$ solves (3.4).

Remark 3.3. The existence of a local solution $H^S_x(\mathbb{R}^2)^2$ to (3.4) is obtained by a standard fixed point argument exploiting the fact that this space is a Banach algebra for $S > 1$ [16, 116]. The choice $S > s+3 > 4$ in the assumptions of Theorem 3.2 is a technical one related to the fact that in their proof Arbunich and Sparber need to compute higher order terms in the multiscale expansion. Moreover, the result proved in [16] is slightly more general, as it is proved that for data *close enough* to spectrally concentrated ones, the dynamics is well approximated by the Dirac system (3.4).

Remark 3.4. In the cubic case the Dirac dynamics is shown to be valid on a time scale $\mathcal{O}(\varepsilon^{-1})$, which is considerably smaller than for the linear case (1.41) where it is of order $\mathcal{O}(\varepsilon^{-2+\delta})$, for all $\delta > 0$. This can be regarded as a nonlinear effect, due to the cubic term in (3.1).

A closely related and interesting problem is the study of the long-time behavior of solutions to nonlinear Dirac equations. However it seems to be quite delicate. Indeed, a major complication to prove global well-posedness is the fact that the energy associated to a solution does not have a definite sign. This is related to the fact that the Dirac spectrum is unboundend on both sides of $\mathbb{R}$. In particular, we are interested in the Cauchy problem for the effective equation (3.12). Recently, Bournaveas and Candy [30] proved global well-posedness of a massless cubic Dirac equation in the critical regularity space $\mathring{H}^{\frac{1}{2}}(\mathbb{R}^2,\mathbb{C}^2)$, for *small* initial data. They deal with *Lorenz-invariant* nonlinearities and their proof relies on the corresponding null-structure, which seems to be absent in our case. This leaves open the problem of global well-posedness, even in the perturbative regime of small data. A further complication is given by the fact that in the massless case the spectral subspaces for the Dirac operator are not separated.

It could be also interesting to study the *massive* variant (3.127), which appear as effective equation for (3.1) in the presence of a suitable perturbation breaking spatial parity (see, e.g. [56, 26]). In that case the existence of stationary solutions can be deduced combining the results of [28, 26]. The global well-posedness for Lorenz-invariant cubic nonlinearities has been treated in [18]. Again, the (apparent) lack of a null-structure of the nonlinear term leaves open the problem for ”positive” nonlinearities, as in (3.127).

We remark that global well-posedness results might be achievable requiring additional (angular) regularity on initial data in order to prove suitable Strichartz estimates, as explained in the survey [34] for the 3-D case and in references therein. Recently the idea of imposing algebraic conditions on initial data has also been investigated, as it might allow to prove GWP for open sets of *large* initial data [37, 42].

3.2 Weakly localized solutions the massless case

The main result presented in this section is contained in the paper [28].

We are interested in studying zero-modes of (3.4) for $\kappa = -1$, that is, we look for particular stationary solutions of the form

$$\psi(t,x) = \psi(x), \qquad (t,x) \in \mathbb{R} \times \mathbb{R}^2.$$

It will turn out that they are in general weakly localized, as they are not even square-integrable, in contrast to the results mentioned for the evolution problem. We expect those zero-modes to be useful to prove approximation results for stationary solutions to (3.1) in the *focusing case* $\kappa = -1$, analogous to the ones proved in [57],[16] for the evolution problem, somehow in the spirit of [70]. Indeed, recall that the energy of a Dirac point $\mu_* \in \sigma{-\Delta + V}$ corresponds to the zero-energy for the Dirac operator $0 \in \sigma(\mathcal{D})$, that is, to the vertex of the cone. Looking for a stationary solution

$$u(t,x) = e^{-i\mu_* t} w(x),$$

one has to study the stationary NLS equation for the profile w

$$(-\Delta + V - \mu_*)\, w = -\kappa |w|^2 w. \tag{3.9}$$

It is then natural make an ansatz of the form

$$w(x) = \sqrt{\varepsilon} \sum_{j=1}^{2} \psi_j(\varepsilon x)\Phi_j(x) + \eta^\varepsilon(x), \qquad \varepsilon > 0, \quad x \in \mathbb{R}^2, \tag{3.10}$$

analogous to the time-dependent case. Then the effective equation solved by the coefficients ψ_j will be the stationary version of (3.4).

However, the rigorous justification of the ansatz (3.10) seem to be a delicate task, as the absence of a gap at the Dirac point is a serious problem to deal with. This will be the object of a future investigation and will be addressed elsewhere. The first step of this program consists in the study of the effective equation for the modulation coefficients, as presented in this section.

As shown in the next section, the amplitudes ψ_j satisfy the following system

$$\begin{cases} \overline{\lambda_\#}(\partial_{x_1}+i\partial_{x_2})\psi_2 = i(2\beta_2|\psi_1|^2+\beta_1|\psi_2|^2)\psi_1 \\ \lambda_\#(\partial_{x_1}-i\partial_{x_2})\psi_1 = i(\beta_1|\psi_1|^2+2\beta_2|\psi_2|^2)\psi_2 \end{cases} \tag{3.11}$$

Moreover, we can easily get rid of $\lambda_\# \neq 0$. Indeed, setting

$$\psi_1(x) = \frac{1}{|\lambda_\#|}\tilde{\psi}_1(x), \quad \psi_2(x) = \frac{\lambda_\#}{|\lambda_\#|^2}\tilde{\psi}_2(x), \qquad x \in \mathbb{R}^2$$

and defining

$$\tilde{\beta}_j := \frac{\beta_j}{|\lambda_\#|^3}, \quad j = 1{,}2,$$

one ends up (dropping superscripts) with the system:

$$\begin{cases} (\partial_{x_1}+i\partial_{x_2})\psi_2 = i(2\beta_2|\psi_1|^2+\beta_1|\psi_2|^2)\psi_1 \\ (\partial_{x_1}-i\partial_{x_2})\psi_1 = i(\beta_1|\psi_1|^2+2\beta_2|\psi_2|^2)\psi_2 \end{cases} \tag{3.12}$$

where $0 < \beta_2 \leqslant \beta_1$, as in (3.5).

For simplicity, we state our main result in terms of equation (3.12).

Theorem 3.5. *(Existence of weakly localized states [28]) Equation (3.12) admits a family of solutions $\psi \in \mathring{H}^{\frac{1}{2}} \cap C^\infty(\mathbb{R}^2,\mathbb{C}^2)$ of the form*

$$\psi(r,\vartheta) = \begin{pmatrix} iu(r)e^{i\vartheta} \\ v(r) \end{pmatrix} \tag{3.13}$$

with $u,v : [0,+\infty) \longrightarrow \mathbb{R}$, (r,ϑ) being polar coordinates in $\mathbb{R}^2$.

Moreover, the spinor components satisfy

$$u(r)v(r) > 0, \qquad \forall r > 0, \tag{3.14}$$

and there holds

$$|u(r)| \sim \frac{1}{r}, \quad |v(r)| \sim \frac{1}{r^2}, \qquad as \quad r \to +\infty, \tag{3.15}$$

In particular,

$$\psi \in L^p(\mathbb{R}^2, \mathbb{C}^2), \quad \forall p > 2,$$

but

$$\psi \notin L^2(\mathbb{R}^2, \mathbb{C}^2).$$

For this reason, we say that those solutions are weakly localized.

Remark 3.6. Heuristically, weak localization is expected as the L^2-spectrum of the massless Dirac operator is equal to $\mathbb{R}$, as it is easily seen using the Fourier transform (see [118] for more details). As shown in Theorem 4.3, in general stationary solutions in the massless case only exhibit a polynomial decay at infinity. This is in striking contrast with the massive case, where stationary solutions (of arbitrary fom) are exponentially localized (see, e.g., [31] where the method of [23] has been generalized to deal with nonlinear bound states in any dimensions).

Remark 3.7. Equation (3.12) is invariant by scaling. Indeed, it can be easily checked that if ψ is a solution, then the same holds for the rescaled spinor

$$\psi_\delta(\cdot) := \sqrt{\delta}\psi(\delta\cdot), \qquad \forall \delta > 0. \tag{3.16}$$

Thus it suffices to prove the existence of one (non-trivial) solution, to get multiplicity. Observe also that if ψ solves the equation, then

$$\tilde{\psi}(\cdot) := -\psi(\cdot) \tag{3.17}$$

is another solution.

Remark 3.8. Theorem 4.3 is in some sense suggested by the literature on the spinorial Yamabe problem. A particular family of test spinors is used to study conformal invariants or nonlinear Dirac equations on spin manifolds (see e.g. [15],[72] and references therein). It is given by

$$\varphi(y) = f(y)(1 - y) \cdot \varphi_0 \qquad y \in \mathbb{R}^2 \tag{3.18}$$

where $\varphi_0 \in \mathbb{C}^2$, $f(y) = \frac{2}{1+|y|^2}$ and the dot represents the Clifford product.

It can be easily checked that these spinors are $\mathring{H}^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2)$-solutions to the following "isotropic" Dirac equation (corresponding to $\beta_1 = 1, \beta_2 = \frac{1}{2}$)

$$\mathcal{D}\varphi = |\varphi|^2\varphi \tag{3.19}$$

The spin structure of euclidean spaces is quite explicit and the spinors in (3.18) can be rewritten in matrix notation as

$$\varphi(y) = f(y)(\mathbb{1}_2 + iy_1\sigma_1 + iy_2\sigma_2) \cdot \varphi_0 \qquad y \in \mathbb{R}^2$$

$\mathbb{1}_2$ and σ_i being the identity and the Pauli matrices, respectively. See [73] for more details. One can show that (3.174) is of the form (4.2.1) and has the decay properties stated in Theorem 3.5.

The present section is organized as follows. The effective equation (3.12) is derived in the next section. Then in Section 3.2.2 we prove Theorem 3.5, exploiting a particular radial ansatz. The proof follows by direct dynamical systems arguments. Then we show in (Section 3.2.3) that the solutions found in the first part of the section admit a variational characterization as $\mathring{H}^{\frac{1}{2}}$-critical points of a suitable functional. This is done using duality, combined with standard concentration compactness theory and Nehari manifold arguments.

3.2.1 Formal derivation

The aim of this subsection is to formally derive the effective Dirac equation (3.12) governing the amplitudes ψ_j appearing in (3.2). To this aim we will perform a multiscale expansion (see e.g. [70, 16, 2]). Since the coefficients $\psi_j(\varepsilon x)$ and the Bloch functions $\Phi_j(x)$ vary on different scales, one can consider x and $y := \varepsilon x, 0 < \varepsilon \ll 1$ as independent variables. Moreover, we look for solution to (3.9) as formal power series in ε, as follows

$$u_\varepsilon = \sqrt{\varepsilon}U_\varepsilon(x,y), \qquad U_\varepsilon(x,y) = U_0(x,y) + \varepsilon U_1(x,y) + \varepsilon^2 U_2(x,y) + ... \tag{3.20}$$

We moreover impose K-pseudoperiodicity with respect to x, i.e.

$$U_\varepsilon(x+v,y) = e^{-iK\cdot v}U_\varepsilon(x,y), \qquad \forall v \in \Lambda, x,y \in \mathbb{R}^2. \tag{3.21}$$

Similarly, we look for μ_ε of the form

$$\mu_\varepsilon = \mu_* + \varepsilon\mu_1 + \varepsilon^2\mu_2 + ... \tag{3.22}$$

Rewriting (3.9) in terms of U_ε and μ_ε then gives

$$\Big(-(\nabla_x+\varepsilon\nabla_y)^2+V(x)-\mu_\varepsilon\Big)\,U_\varepsilon(x,y)=\varepsilon\,|U_\varepsilon(x,y)|^2\,U_\varepsilon(x,y). \tag{3.23}$$

Plugging (3.20,3.22) into (3.23) one finds a hierarchy of equations corresponding to the different powers of ε in the expansion. In particular, one obtains at order $\mathcal{O}(\varepsilon^0)$

$$(-\Delta_x+V-\mu_*)U_0=0. \tag{3.24}$$

Recall that $\ker_{L^2_K}(-\Delta+V-\mu_*)=\operatorname{Span}\{\Phi_1,\Phi_2\}$, and then by (3.21) we have

$$U_0(x,y)=\psi_1(y)\Phi_1(x)+\psi_2(y)\Phi_2(x), \tag{3.25}$$

where the amplitudes are to be determined solving the next equation in the formal expansion. Looking at the equation for $\mathcal{O}(\varepsilon)$ terms one finds

$$(-\Delta_x+V-\mu_*)U_1=(2\nabla_x\cdot\nabla_y+\mu_1)\,U_0+|U_0|^2\,U_0. \tag{3.26}$$

By Fredholm alternative [32], in order to solve the above equation, its right hand side must be L^2-orthogonal to the kernel of $(-\Delta_x+V-\mu_*)$. Then the amplitudes ψ_j are determined imposing orthogonality to the Bloch functions Φ_k. For simplicity we deal with linear part and the cubic term in the right hand side of (3.26) separately.

The linear terms can be calculated using the following lemma from [56]

Lemma 3.9. *Let $\zeta=(\zeta_1,\zeta_2)\in\mathbb{C}^2$ be a vector. Then we have*

$$\begin{aligned}
&\langle\Phi_k,\zeta\cdot\nabla\Phi_k\rangle_{L^2(\Omega)}=0,\qquad k=1{,}2,\\
&2i\langle\Phi_1,\zeta\cdot\nabla\Phi_2\rangle_{L^2(\Omega)}=\overline{2i\langle\Phi_2,\zeta\cdot\nabla\Phi_1\rangle_{L^2(\Omega)}}=-\overline{\lambda_\#}\,(\zeta_1+i\zeta_2)\,,\\
&2i\langle\Phi_2,\zeta\cdot\nabla\Phi_1\rangle_{L^2(\Omega)}=-\lambda_\#(\zeta_1-i\zeta_2)
\end{aligned} \tag{3.27}$$

Notice that $(\nabla_x\cdot\nabla_y)\,U_0=\sum_{j=1}^2\nabla_y\psi_j\cdot\nabla_x\Phi_j$ and then applying Lemma 3.9 with $\zeta=\nabla_y\Phi_j, j=1{,}2$ we get

$$\begin{aligned}
&2i\langle\Phi_1,\nabla_y\psi_2\cdot\nabla\Phi_2\rangle_{L^2(\Omega)}=\overline{2i\langle\Phi_2,\nabla_y\psi_2\cdot\nabla\Phi_1\rangle_{L^2(\Omega)}}=-\overline{\lambda_\#}\,(\partial_{y_1}+i\partial_{y_2})\,\psi_2,\\
&2i\langle\Phi_2,\nabla_y\psi_1\cdot\nabla\Phi_1\rangle_{L^2(\Omega)}=-\lambda_\#(\partial_{y_1}-i\partial_{y_2})\psi_1
\end{aligned} \tag{3.28}$$

Thus we see that taking the $L^2(\Omega)$ scalar product of the linear part in the right hand side of (3.26) with the Bloch functions Φ_j gives the linear part of (3.11). We now want to show that the cubic nonlinearity in (3.11) is obtained calculating the same product for the cubic term in (3.26). A symmetry argument allows to show that taking this projection many terms vanish. The cubic term reads as

$$|U_0|^2 U_0 = \sum_{1\leqslant j,k,l\leqslant 2} \psi_j\psi_k\overline{\psi_k}\Phi_j\Phi_k\overline{\Phi_l}. \tag{3.29}$$

Let us consider, for instance, the term $\psi_1\psi_1\overline{\psi_2}\Phi_1\Phi_1\overline{\Phi_2}$ and then project it onto Φ_1. We compute

$$\begin{aligned}\langle\Phi_1, \Phi_1\Phi_1\overline{\Phi_2}\rangle_{L^2(\Omega)} &= \int_\Omega \overline{\Phi_1(x)}\Phi_1(x)\Phi_1(x)\overline{\Phi_2(x)}dx \\ &=^{x=R^*y} \int_{R\Omega} \overline{\Phi_1(R^*y)}\Phi_1(R^*y)\Phi_1(R^*y)\overline{\Phi_2(R^*y)}dy \\ &\int_{R\Omega} \overline{\tau\Phi_1(y)}\tau\Phi_1(y)\tau\Phi_1(y)\overline{\overline{\tau}\Phi_2(y)}dy \\ &\tau^2 \int_\Omega \overline{\Phi_1(x)}\Phi_1(x)\Phi_1(x)\overline{\Phi_2(x)}dx = \tau^2\langle\Phi_1, \Phi_1\Phi_1\overline{\Phi_2}\rangle_{L^2(\Omega)}\end{aligned} \tag{3.30}$$

where R is the rotation matrix (1.15), recalling that $\mathcal{R}\Phi_1 = \tau\Phi_1$ and $\mathcal{R}\Phi_2 = \overline{\tau}\Phi_2$, see (1.29,1.28). We see from (3.30) that

$$(1-\tau^2)\langle\Phi_1, \Phi_1\Phi_1\overline{\Phi_2}\rangle_{L^2(\Omega)} = 0,$$

and thus

$$\langle\Phi_1, \Phi_1\Phi_1\overline{\Phi_2}\rangle_{L^2(\Omega)} = 0.$$

Iterating this calculations one can check that

$$\begin{cases} \langle\Phi_1, |U_0|^2 U_0\rangle_{L^2(\Omega)} = (2\beta_2|\psi_1|^2 + \beta_1|\psi_2|^2)\psi_1 \\ \langle\Phi_2, |U_0|^2 U_0\rangle_{L^2(\Omega)} = (\beta_1|\psi_1|^2 + 2\beta_2|\psi_2|^2)\psi_2 \end{cases} \tag{3.31}$$

thus recovering the cubic term in (3.11), with

$$\beta_1 := \int_\Omega |\Phi_1|^4 dx = \int_\Omega |\Phi_2|^4 dx, \qquad \beta_2 := \int_\Omega |\Phi_1|^2|\Phi_2|^2. \tag{3.32}$$

It is then easy to see that (3.11) appears as compatibility condition for the solvability of (3.26), combining (3.28, 3.31) and taking $\mu_1 = 0$ in (3.26).

3.2.2 Existence and asymptotics

In this section we prove Theorem (4.3), providing the existence and the exact asymptotic behavior of (non-trivial) solutions of (3.12) satisfying the ansatz (4.2.1). The latter allows us to convert the PDE (3.12) into a dynamical system. Indeed, passing to polar coordinates in $\mathbb{R}^2$, $(x_1, x_2) \mapsto (r, \vartheta)$, the equation reads as:

$$\begin{cases} -e^{i\vartheta}\left(i\partial_r - \dfrac{\partial_\vartheta}{r}\right)\psi_2 = -\left(2\beta_2|\psi_1|^2 + \beta_1|\psi_2|^2\right)\psi_1, \\ -e^{-i\vartheta}\left(i\partial_r + \dfrac{\partial_\vartheta}{r}\right)\psi_1 = \left(\beta_1|\psi_1|^2 + 2\beta_2|\psi_2|^2\right)\psi_2. \end{cases} \tag{3.33}$$

Plugging the ansatz

$$\psi(r, \vartheta) = \begin{pmatrix} iu(r)e^{i\vartheta} \\ v(r) \end{pmatrix} \tag{3.34}$$

into (3.33) gives:

$$\begin{cases} \dot{u} + \dfrac{u}{r} = v(2\beta_2 u^2 + \beta_1 v^2) \\ \dot{v} = -u(\beta_1 u^2 + 2\beta_2 v^2) \end{cases} \tag{3.35}$$

Thus we are led to study the flow of the above system.

In particular, since we are looking for localized states, we are interested in solutions to (3.35) such that

$$(u(r), v(r)) \longrightarrow (0{,}0) \qquad \text{as} \qquad r \to +\infty$$

In order to avoid singularities and to get non-trivial solutions, we choose as initial conditions

$$u(0) = 0 \quad , \quad v(0) = \lambda \neq 0 \tag{3.36}$$

Moreover, the symmetry of the system allows us to consider only the case $\lambda > 0$. Thus (Theorem 4.3) reduces to the following

Proposition. *For any* $\lambda > 0$ *there exists a unique solution*

$$(u_\lambda, v_\lambda) \in C^\infty([0, +\infty), \mathbb{R}^2)$$

of the Cauchy problem (3.35,3.36).

Moreover, there holds

$$u_\lambda(r), v_\lambda(r) > 0, \qquad \forall r > 0, \tag{3.37}$$

and

$$u_\lambda(r) \sim \frac{1}{r}, \quad v_\lambda(r) \sim \frac{1}{r^2}, \qquad as \quad r \to +\infty, \tag{3.38}$$

In particular,

$$\psi \in L^p(\mathbb{R}^2, \mathbb{C}^2), \quad \forall p > 2,$$

but

$$\psi \notin L^2(\mathbb{R}^2, \mathbb{C}^2).$$

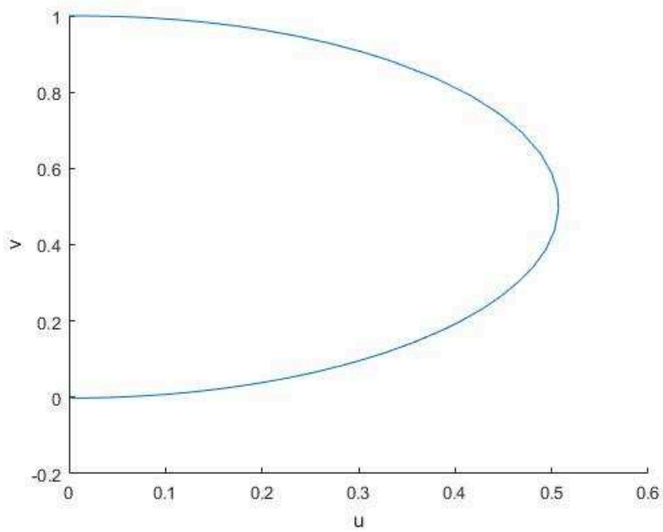

Figure 3.1. The trajectory of a representative solution of (3.35) with $\lambda > 0$.

The proof of (Prop. 3.3.3) will be achieved in several intermediate steps.

Local existence and uniqueness of solutions of (3.35) are guaranteed by the following

Lemma 3.10. *Let* $\lambda > 0$*. There exist* $0 < R_\lambda \leqslant +\infty$ *and* $(u, v) \in C^1([0, R_\lambda), \mathbb{R}^2)$ *unique maximal solution to (3.35), which depends continuously on* λ *and uniformly on* $[0, R]$ *for any* $0 < R < R_\lambda$.

Proof. We can rewrite the system in integral form as

$$\begin{cases} u(r) = \dfrac{1}{r}\displaystyle\int_0^r sv(s)(2\beta_2 u^2(s) + \beta_1 v^2(s))ds \\ v(r) = \lambda - \displaystyle\int_0^r u(s)(\beta_1 u^2(s) + 2\beta_2 v^2(s))ds \end{cases} \tag{3.39}$$

where the r.h.s. is a Lipschitz continuous function with $(u, v) \in C^1$. Then the claim follows by a contraction mapping argument, as in [40]. □

Given $\lambda > 0$, we will denote by (u_λ, v_λ) the corresponding (maximal) solution. Dropping the singular term in (3.35) we obtain a hamiltonian system

$$\begin{cases} \dot{u} = v(2\beta_2 u^2 + \beta_1 v^2) \\ \dot{v} = -u(\beta_1 u^2 + 2\beta_2 v^2) \end{cases} \tag{3.40}$$

whose hamiltonian is given by

$$H(u,v) = \frac{\beta_1}{4}(u^4 + v^4) + \beta_2 u^2 v^2 \tag{3.41}$$

Consider

$$H_\lambda(r) := H(u_\lambda(r), v_\lambda(r)) \tag{3.42}$$

then a simple computation gives

$$\dot{H}_\lambda(r) = -\frac{u_\lambda^2(r)}{r}(\beta_1 u_\lambda^2(r) + 2\beta_2 v_\lambda^2(r)) \leqslant 0 \tag{3.43}$$

so that the energy H is non-increasing along the solutions of (3.35).

This implies that $\forall r \in [0, R_x)$, $(u_\lambda(r), v_\lambda(r)) \in \{H(u,v) \leqslant H(0,\lambda)\}$, the latter being a compact set. Thus there holds

Lemma 3.11. *Every solution to (3.35) is global.*

Remark 3.12. Smoothness of solutions follows by basic ODE theory.

Heuristically, (3.35) should reduce to (3.40) in the limit $r \to +\infty$ (u being bounded), that is, dropping the singular term in the first equation. The following lemma indeed shows that the solutions to (3.35) are close to the hamiltonian flow (3.40) as $r \to +\infty$. The proof is the same as in [40].

Lemma 3.13. *Let (f,g) be the solution of (3.40) with initial data (f_0, g_0). Let (u_n^0, v_n^0) and ρ_n be such that*

$$\rho_n \xrightarrow{n\to+\infty} +\infty \qquad \textit{and} \qquad (u_n, v_n) \xrightarrow{n\to+\infty} (f_0, g_0)$$

Consider the solution of

$$\begin{cases} \dot{u}_n + \dfrac{u_n}{r+\rho_n} = (2\beta_2 u_n^2 + \beta_1 v_n^2) v_n \\ \qquad\qquad \dot{v}_n = -(\beta_1 u_n^2 + 2\beta_2 v_n^2) u_n \end{cases}$$

such that $u_n(0) = u_n^0$ *and* $v_n(0) = v_n^0$. *Then* (u_n, v_n) *converges to* (f, g) *uniformly on bounded intervals.*

Proposition. *For any* $\lambda > 0$*, we have*

$$u_\lambda(r), v_\lambda(r) > 0, \qquad \forall r > 0. \tag{3.44}$$

and

$$\lim_{r\to+\infty} (u_\lambda(r), v_\lambda(r)) = (0{,}0). \tag{3.45}$$

Proof. Using the equations in (3.35) one can compute

$$\frac{d}{dr}(r u_\lambda(r) v_\lambda(r)) = \beta_1 r (v_\lambda^4 - u_\lambda^4), \tag{3.46}$$

and

$$\frac{d}{dr}(r^2 H_\lambda(r)) = \frac{\beta_1}{2} r (v_\lambda^4 - u_\lambda^4). \tag{3.47}$$

Combining (3.46) and (3.47) and integrating gives

$$u_\lambda(r) v_\lambda(r) = 2r H_\lambda(r) \tag{3.48}$$

and (3.44) follows, H_λ being positive definite.

Combining (3.44) and the second equation in (3.35) one sees that $\dot{v}_\lambda(r) \leqslant 0$ for all $r > 0$, and then

$$\exists \lim_{r\to+\infty} v_\lambda(r) =: \mu \geqslant 0. \tag{3.49}$$

Moreover, since u is bounded, there exists a sequecnce $r_n \uparrow +\infty$ such that

$$\exists \lim_{n\to+\infty} u_\lambda(r_n) = \delta \geqslant 0. \tag{3.50}$$

We claim that

$$\lim_{r\to+\infty} u_\lambda(r) = \delta. \tag{3.51}$$

By contradiction, suppose that (3.51) does not hold. Then there exist $\varepsilon > 0$ and another sequence $s_n \uparrow +\infty$ such that

$$|u_\lambda(s_n) - \delta| \geqslant \varepsilon \geqslant 0, \qquad \forall n \in \mathbb{N}. \tag{3.52}$$

Up to subsequences, we can suppose that

$$\lim_{n\to+\infty} u_\lambda(s_n) = \gamma \neq \delta, \tag{3.53}$$

for some $\gamma \geqslant 0$. Recall that H decreases along the flow of (3.35), as shown in (3.43), and then

$$\exists \lim_{r\to+\infty} H_\lambda(r) = h \geqslant 0. \tag{3.54}$$

Then it follows that

$$(\delta,\mu),(\gamma,\mu) \in \{H(u,v) = h\}. \tag{3.55}$$

It is easy to see that the algebraic equation for u

$$H(u,\mu) = h, \tag{3.56}$$

has (at most) one non-negative solution and thus $\delta = \gamma$, reaching a contradiction. This proves the claim (3.51), and then there holds

$$\lim_{r\to+\infty} (u_\lambda(r), v_\lambda(r)) = (\delta,\mu). \tag{3.57}$$

Let $(\rho_n)_n \subseteq \mathbb{R}$ be a sequence such that

$$\lim_{n\to+\infty} \rho_n = +\infty \quad , \quad \lim_{n\to+\infty} (u_\lambda(\rho_n), v_\lambda(\rho_n)) = (\delta,\mu) \tag{3.58}$$

and consider the solution (U,V) to (3.40) such that

$$(U(0),V(0)) = (\delta,\mu).$$

By Lemma 3.28, it follows that $(u_\lambda(\rho_n+\cdot), v_\lambda(\rho_n+\cdot))$ converges uniformly to (U,V) on bounded intervals. But since

$$\lim_{n\to+\infty}(u_\lambda(\rho_n+r),v_\lambda(\rho_n+r))=(\delta,\mu),\qquad \forall r>0, \tag{3.59}$$

this implies that

$$(U(r)),V(r))=(\delta,\mu),\qquad \forall r>0 \tag{3.60}$$

and thus $(\delta,\mu)=(0{,}0)$ as the latter is the only equilibrium of the hamiltonian system (3.40). This proves (3.45). □

The above proposition shows that the solutions of (3.35) actually correspond to localized solutions of the PDE (3.12). The aim of the rest of the section is then to provide the exact asymptotic behavior.

Proposition. *For large $r>0$, there holds*

$$\frac{1}{r^2}\lesssim u_\lambda^2(r)+v_\lambda^2(r)\lesssim\frac{1}{r}. \tag{3.61}$$

Proof. Remark that

$$(u_\lambda^2(r)+v_\lambda^2(r))^2\sim H_\lambda(r). \tag{3.62}$$

Moreover, by (3.150,3.43) one gets

$$\dot H_\lambda(r)\geqslant -4\frac{H_\lambda(r)}{r},$$

and the comparison principle for ODEs implies that

$$H_\lambda(r)\gtrsim\frac{1}{r^4}$$

and thus by (3.151), we get the first inequality in (3.165).

The second part of (3.165) follows by (3.48,3.151), using the elementary inequality

$$2u_\lambda(r)v_\lambda(r)\leqslant u_\lambda^2(r)+v_\lambda^2(r),\qquad \forall r>0.$$

□

The first equation in (3.35) can be rewritten as

$$\frac{d}{dr}(ru_\lambda(r))=rv_\lambda(r)(2\beta_2u_\lambda^2(r)+\beta_1v_\lambda^2(r)) \tag{3.63}$$

Since $v_\lambda > 0$, we deduce from (3.63) that the function $f(r) := (ru_\lambda(r))$ is strictly increasing and thus

$$\lim_{r\to+\infty} f(r) =: l \in (0,+\infty] \tag{3.64}$$

Suppose that

$$l = +\infty. \tag{3.65}$$

This implies that

$$u_\lambda(r) \geqslant \frac{1}{r} \tag{3.66}$$

for $r > 0$ large. Combining (3.66) and (3.165), using the second equation in (3.35) we deduce that

$$\dot{v}_\lambda(r) \lesssim -\frac{1}{r^3}. \tag{3.67}$$

Using again the comparison principle, we conclude that

$$v_\lambda(r) \lesssim \frac{1}{r^2} \tag{3.68}$$

for $r > 0$ large. By (3.165,3.68), integrating (3.63) gives

$$f(r) = \int_0^r v_\lambda(s)\,\underbrace{(2\beta_2 u_\lambda^2(s) + \beta_1 v_\lambda^2(s))s}_{bounded}\,ds \lesssim \int_0^{+\infty} \frac{ds}{s^2} < +\infty, \quad \forall r > 0, \tag{3.69}$$

thus contradicting (3.65). Then $0 < l < +\infty$, and this implies that

$$u_\lambda(r) \sim \frac{1}{r} \tag{3.70}$$

for large $r > 0$. Since (3.68) holds, using the second equation in (3.35) and (3.70) one gets

$$\dot{v}_\lambda(r) \sim -\frac{1}{r^3}. \tag{3.71}$$

and then for large $r > 0$, we have

$$v_\lambda(r) \sim \frac{1}{r^2}. \tag{3.72}$$

The integrability properties of the solution follow by the fact that

$$|\psi(r)|^2 = u_\lambda^2(r) + v_\lambda^2(r) \sim \frac{1}{r^2},$$

as $r \longrightarrow +\infty$. This concludes the proof of (Prop. 3.3.3), and thus of (Theorem 4.3).

3.2.3 Variational characterization

The solutions of (3.12) found in the previous section by dynamical systems methods admit a variational characterization. Indeed, one can prove that they are critical points of a suitable action functional. More precisely one can show that they are *least action* critical points of the corresponding action. In this sense they can be considered as *ground state solutions*. Our variational argument also provides an alternative, more sophisticated, existence proof. This is not only interesting in itself, but also gives more information about the properties of those solutions.

Remark 3.14. The argument presented in this section works for $\mathring{H}^{\frac{1}{2}}$-solutions of (3.73) of arbitrary form. However, we focus on symmetric solutions of the form (4.2.1) as in that case we can also provide the exact asymptotic behavior of solutions, by the method described in the previous section.

Theorem 3.15. *Equation (3.12) admits a family of smooth solutions in $\mathring{H}^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2)$, of the form (4.2.1) and satisfying the decay estimates (3.31). Moreover, they coincide with the solutions found in the previous section (Theorem 4.3).*

This section is devoted to the proof of the above theorem. Some preliminary definitions are in order.

The system (3.12) can be written in a more compact form as:

$$\mathcal{D}\psi = \nabla G_{\beta_1,\beta_2}(\psi), \tag{3.73}$$

with $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} : \mathbb{R}^2 \longrightarrow \mathbb{C}^2$, where

$$G_{\beta_1,\beta_2}(\psi) := \frac{\beta_1}{4}(|\psi_1|^4 + |\psi_2|^4) + \beta_2|\psi_1|^2|\psi_2|^2. \tag{3.74}$$

To simplify notations, in the sequel we omit the indices β_j.

Here

$$\mathcal{D} := -i(\vec{\sigma} \cdot \nabla) \tag{3.75}$$

is the Dirac operator and $\vec{\sigma} \cdot \nabla := \tilde{\sigma}_1 \partial_1 + \tilde{\sigma}_2 \partial_2$, where

$$\tilde{\sigma}_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \tilde{\sigma}_2 := \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \tag{3.76}$$

are Pauli-type matrices[1].

It is easy to see that (3.73) is, formally, the Euler-Lagrange equation of the action functional

$$\mathcal{L}(\psi) := \frac{1}{2} \int_{\mathbb{R}^2} \langle \psi, \mathcal{D}\psi \rangle dx - \int_{\mathbb{R}^2} G(\psi) dx. \tag{3.77}$$

We look for critical points of (5.22) belonging to the Sobolev space $\mathring{H}^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2)$, as this is a natural choice in view of the continuous embedding

$$\mathring{H}^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2) \hookrightarrow L^4(\mathbb{R}^2, \mathbb{C}^2). \tag{3.78}$$

given by the Gagliardo-Nirenberg inequality (see, e.g.[55]). Moreover, it is not hard to see that $\mathcal{L} \in C^1(\mathring{H}^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2))$.

More precisely, we will work with the closed subspace of functions satisfying (4.2.1):

$$E := \left\{ \psi \in \mathring{H}^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2) : \psi(r, \vartheta) = \begin{pmatrix} iu(r)e^{i\vartheta} \\ v(r) \end{pmatrix}, u, v : [0, +\infty) \longrightarrow \mathbb{R} \right\}, \tag{3.79}$$

(r, ϑ) being polar coordinates in $\mathbb{R}^2$. To simplify the presentation, we will sometimes adopt the notation

$$\psi = (u, v) \tag{3.80}$$

for $\psi \in E$, and more generally for spinors satisfying (4.2.1). We will often identify ψ with the pair (u, v).

If $\psi \in E$, the action functional on E reads as

$$\mathcal{S}(u, v) = \frac{\mathcal{L}(\psi)}{2\pi} = \int_0^{+\infty} \left(\frac{1}{2} \left(\dot{u}v + \frac{uv}{r} - u\dot{v} \right) - H(u, v) \right) r dr \tag{3.81}$$

---

[1] We could rewrite the equation (3.12) in terms of standard Pauli matrices $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. This amounts to an unitary transformation on the spinor space $\mathbb{C}^2$ and does not affect our argument. However we prefer not to do so, in order to remain consistent with the notations of [16].

where H is the hamiltonian defined in (3.150). It is not hard to see that the Euler-Lagrange equation for (3.81) is given by the ODE (3.35).

Looking for critical points of (3.81) one may try to prove that it has a linking geometry (see e.g. in [54]). However, since this may not be straightforward we rather exploit the convexity of the hamiltonian H in order to use duality techniques. This allows us to easily define a minimax level, the dual functional possessing a mountain pass structure. Duality is a classical tool in the study of hamiltonian systems (see [89, 47]), which turns out to be useful also for elliptic PDEs as shown, for instance, in [72, 12].

Lemma 3.16. *The function*

$$H : (u, v) \in \mathbb{R}^2 \longrightarrow H(u, v) \in \mathbb{R}$$

is convex.

Proof. A simple computation gives

$$\det D^2 H(u, v) = 6\beta_1\beta_2(u^4 + v^4) + (9\beta_2^1 - 12\beta_2^2)u^2v^2. \tag{3.82}$$

Recall that $0 < \beta_2 \leqslant \beta_1$, and then by (3.82)

$$\det D^2 H(u, v) > \beta_2^2 \left[6(u^4 + v^4) - 3u^2v^2\right] > \frac{9}{2}\beta_2^2(u^4 + v^4) \tag{3.83}$$

thanks to the elementary inequality $2u^2v^2 \leqslant u^4 + v^4$, and the claim follows. □

We can thus define the *Legendre transform* $H^* : \mathbb{R}^2 \longrightarrow \mathbb{R} \cup \{+\infty\}$ of H as the function

$$H^*(w, z) = \sup\{\langle (u, v), (w, z)\rangle_{\mathbb{R}^2} - H(u, v) \ : \ (u, v) \in \mathbb{R}^2\} \tag{3.84}$$

The hamiltonian H is a homogeneous polynomial of degree 4. This implies that H^* is everywhere finite and, thanks to basic scaling properties of the Legendre transform, it is homogeneous of degree $\frac{4}{3}$. Moreover, since $H(0{,}0) = 0$, it immediately follows from (3.84) that H^* is positive definite. We collect those remarks in the following

Proposition. *The function H^* is everywhere finite, positive definite and homogeneous of degree $\frac{4}{3}$.*

Consider the functional, defined for $(u, v) \in L^4(\mathbb{R}_+, rdr)^2$ as

$$\mathcal{H}(u, v) := \int_0^{+\infty} H(u, v) r dr \tag{3.85}$$

Its Legendre transform (or dual) is the functional

$$\mathcal{H}^* : L^{\frac{4}{3}}(\mathbb{R}_+, rdr)^2 \longrightarrow \mathbb{R} \tag{3.86}$$

defined (with an abuse of notation) as

$$\begin{aligned} \mathcal{H}^*(w,z) &:= \sup\{\langle (u,v),(w,z)\rangle_{L^4 \times L^{\frac{4}{3}}} - \mathcal{H}(u,v) \ : \ (u,v) \in L^4(\mathbb{R}_+, rdr)^2\} \\ &= \int_0^{+\infty} H^*(w,z) rdr \end{aligned} \tag{3.87}$$

where $\langle \cdot, \cdot \rangle_{L^4 \times L^{\frac{4}{3}}}$ stands for the duality product. There holds

$$d\mathcal{H} \circ d\mathcal{H}^* = \mathrm{id}_{L^{\frac{4}{3}}}, \quad d\mathcal{H}^* \circ d\mathcal{H} = \mathrm{id}_{L^4}. \tag{3.88}$$

Consider the following isomorphism

$$\mathcal{D} : E \longrightarrow E^*, \tag{3.89}$$

and its inverse

$$A := \mathcal{D}^{-1} : E^* \longrightarrow E. \tag{3.90}$$

where E^* is the dual of E. Let

$$j : E \longrightarrow L^4(\mathbb{R}_+, rdr)^2 \tag{3.91}$$

be the Sobolev embedding. Consider the following sequence of maps

$$K : L^{\frac{4}{3}}(\mathbb{R}_+, rdr)^2 \xrightarrow{j^*} E^* \xrightarrow{A} E \xrightarrow{j} L^4(\mathbb{R}_+, rdr)^2, \tag{3.92}$$

The action functional (3.81) can be rewritten as

$$\mathcal{S}(u,v) = \frac{1}{2}\langle (w,z), \mathcal{D}(w,z)\rangle_{E \times E'} - \mathcal{H}(j(u,v)), \qquad (u,v) \in E. \tag{3.93}$$

Then for $\psi = (u,v) \in E$ the differential of $\mathcal{S}$ reads as

$$d\mathcal{S}(\psi) = \mathcal{D}\psi - j^* d\mathcal{H}(j(\psi)) \in E^*. \tag{3.94}$$

We finally define the dual action functional

$$\begin{aligned}\mathcal{S}^*(w,z) :&= \mathcal{H}^*(w,z) - \frac{1}{2}\langle K(w,z),(w,z)\rangle_{L^4\times L^{\frac{4}{3}}} \\ &= \int_0^{+\infty} H^*(w,z)rdr - \frac{1}{2}\int_0^{+\infty}\langle K(w,z),(w,z)\rangle rdr\end{aligned} \tag{3.95}$$

for $(w,z)\in L^{\frac{4}{3}}(\mathbb{R}_+,rdr)^2$,which is of class C^1 on $L^{\frac{4}{3}}(\mathbb{R}_+,rdr)^2$.

Proposition. *There is a one-to-one correspondence between critical points of $\mathcal{S}$ in E and critical points of $\mathcal{S}^*$ in $L^{\frac{4}{3}}(\mathbb{R}_+,rdr)^2$.*

Proof. Let $\psi\in E$ be a critical point of S. Then by (3.94), we have $\mathcal{D}\psi = j^* d\mathcal{H}(j(\psi))$. Define $\varphi = d\mathcal{H}(j(\psi))\in L^{\frac{4}{3}}(\mathbb{R}_+,rdr)^2$, so that $\mathcal{D}\psi = j^*(\varphi)$. This implies that $\psi = A\circ j^*(\varphi)$ and

$$j(\psi) = j\circ A\circ j^*(\varphi) = K(\varphi). \tag{3.96}$$

On the other hand, by (3.88) we have

$$j(\psi) = d\mathcal{H}^*(\varphi). \tag{3.97}$$

Combining (3.96) and (3.97) we obtain

$$d\mathcal{S}^*(\varphi) = d\mathcal{H}^*(\varphi) - K(\varphi) = 0, \tag{3.98}$$

and then φ is a critical point of $\mathcal{S}^*$.

Conversely, suppose $\varphi\in L^{\frac{4}{3}}(\mathbb{R}_+,rdr)^2$ is a critical point of $\mathcal{S}^*$, and define $\psi = A\circ j^*(\varphi)\in E$. Since φ is a critical point, we have $d\mathcal{H}^*(\varphi) - K(\varphi) = 0$. Then (3.88) implies that

$$\varphi = d\mathcal{H}\circ K(\varphi) = d\mathcal{H}\circ j\circ A\circ j^*(\varphi) = d\mathcal{H}(j(\psi)). \tag{3.99}$$

We have $j^*(\varphi) = j^*\circ d\mathcal{H}(j(\psi))$ and $\mathcal{D}\psi = j^*\circ d\mathcal{H}(j(\psi))$, and thus ψ is a critical point of $\mathcal{S}$. □

Remark 3.17. More generally, $\mathcal{S}$ and $\mathcal{S}^*$ have the same compactness properties and there is a one-to-one correspondence between their Palais-Smale sequences (see, e.g. [72] for more details).

Since finding a critical point of $\mathcal{S}$ is equivalent to finding a critical point of the dual functional $\mathcal{S}^*$ we will focus on the latter, which has a simpler structure. More precisely, we will exploit the homogeneity properties of $\mathcal{S}^*$ using a Nehari-manifold argument (see, e.g. [115] and references therein). However, the fact that the second integral in (3.95) is not positive definite must be taken into account. We remark that a Nehari-type argument has been previously used by Ding and Ruf [43], in the study of semiclassical states for critical Dirac equations.

We have pointed out (Remark 3.7) that the equation (3.73), and thus the functional (5.22), is scale-invariant. The same holds, of course, for the dual action $\mathcal{S}^*$. Indeed, one can verify that it is invariant with respect to the following scaling

$$\psi(\cdot) \mapsto \psi_\delta(\cdot) := \delta^{\frac{3}{2}}\psi(\delta\cdot), \quad \delta > 0. \tag{3.100}$$

Moreover, even if the functional (5.22) is invariant by translation, this is no longer true for (3.95) thanks to the ansatz (4.2.1). Thus scaling is the only (local) symmetry which may prevent strong convergence in our variational procedure. In what follows we only sketch the rest of the proof, as it is based on standard arguments from concentration-compactness theory [84, 85, 114].

First of all, it easy to see that the functional $\mathcal{S}^*$ possesses a mountain-pass geometry.

Lemma 3.18. *There exists $\rho > 0$ such that*

$$\alpha := \inf\{\mathcal{S}^*(w,z) \ : \ (w,z) \in L^{\frac{4}{3}}(\mathbb{R}_+, rdr)^2, \ \|(w,z)\|_{\frac{4}{3}} = \rho\} > 0.$$

Moreover, for $(w,z) \in L^{\frac{4}{3}}(\mathbb{R}_+, rdr)^2$ such that $\int_0^{+\infty}\langle K(w,z),(w,z)\rangle rdr > 0$, there holds

$$\lim_{t\to+\infty} \mathcal{S}^*(t(w,z)) = -\infty.$$

Proof. Recall that the dual functional is defined as

$$\mathcal{S}^*(w,z) = \int_0^{+\infty} H^*(w,z)rdr - \frac{1}{2}\int_0^{+\infty}\langle K(w,z),(w,z)\rangle rdr$$

for $(w,z) \in L^{\frac{4}{3}}(\mathbb{R}_+, rdr)^2$. Since H^* is homogeneous of degree $\frac{4}{3}$, as already remarked, the first assertion follows is $\rho > 0$ is sufficiently small, the other term being quadratic. The second part of the claim follows immediately, for the same reason. □

In view of the above lemma it is natural to define the mountain-pass level for $\mathcal{S}^*$ as

$$c := \inf\left\{\max_{t\geqslant 0}\mathcal{S}^*(t(w,z)) \ : \ (w,z) \in L^{\frac{4}{3}}(\mathbb{R}_+, rdr)^2, \int_0^{+\infty}\langle K(w,z),(w,z)\rangle rdr > 0\right\}.$$

Remark that there holds

$$\max_{t\geqslant 0}\mathcal{S}^*(t(w,z))\geqslant\alpha>0,\qquad\forall(w,z)\in L^{\frac{4}{3}}(\mathbb{R}_+,rdr)^2,\tag{3.101}$$

where $\alpha>0$ is as in Lemma 3.18. Then we have

$$c\geqslant\alpha>0.\tag{3.102}$$

Moreover, the homogeneity properties of the terms appearing in $\mathcal{S}^*$ imply that

$$c=\inf_{(w,z)\in\mathcal{N}}\mathcal{S}^*(w,z)>0,\tag{3.103}$$

where $\mathcal{N}$ is the Nehari manifold

$$\mathcal{N}:=\{(w,z)\in L^{\frac{4}{3}}(\mathbb{R}_+,rdr)^2\setminus\{0\}:\langle d\mathcal{S}^*(w,z),(w,z)\rangle=0\}.\tag{3.104}$$

We are thus led to study the minimization problem (3.103).

Let $(w_n,z_n)_{n\in\mathbb{N}}\subseteq\mathcal{N}$ be a minimizing sequence for $\mathcal{S}^*$. By Ekeland's variational principle (see [47]), we can assume that it actually is a Cerami-sequence, that is:

$$\begin{cases}\mathcal{S}^*(w_n,z_n)\longrightarrow c,\\ (1+\|(w_n,z_n)\|_{L^{\frac{4}{3}}})d\mathcal{S}^*(w_n,z_n)\xrightarrow{L^4}0,\end{cases}\qquad\text{as}\quad n\longrightarrow\infty.\tag{3.105}$$

Proposition. *The sequence $(w_n,z_n)_{n\in\mathbb{N}}\subseteq\mathcal{N}$ is bounded in $L^{\frac{4}{3}}(\mathbb{R}_+,rdr)^2$.*

Proof. We have

$$d\mathcal{S}^*(w_n,z_n)=\nabla H^*(w_n,w_n)-K(w_n,z_n).$$

Since the function H^* is $\frac{4}{3}$-homogeneous there holds

$$\langle\nabla H^*(w_n,w_n),(w_n,z_n)\rangle=\frac{4}{3}H^*(w_n,z_n).$$

Then by the definition of the Nehari manifold (3.104), it follows that

$$\mathcal{S}^*(w_n,z_n)=\frac{1}{3}\int_0^{+\infty}H^*(w_n,z_n)rdr.\tag{3.106}$$

The claim thus follows because

$$\int_0^{+\infty}H^*(w_n,z_n)rdr\sim\|(w_n,z_n)\|^{\frac{4}{3}}_{L^{\frac{4}{3}}},\tag{3.107}$$

and $(w_n, z_n)_{n\in\mathbb{N}}$ is a minimizing sequence. $\square$

By the above lemma we may assume that

$$(w_n, z_n) \rightharpoonup (w, z), \qquad \text{weakly in} \quad L^{\frac{4}{3}}(\mathbb{R}_+, rdr)^2, \tag{3.108}$$

as $n \to +\infty$. One needs to study the concentration behavior of the minimizing sequence in order to prove *strong* $L^{\frac{4}{3}}$-convergence.

We already remarked that scaling invariance may prevent strong convergence, as Cerami sequences may blow-up around some points. Since we are essentially working with radial functions, concentration may only occur at the origin. More precisely (recall (3.107)), there holds

$$H^*(w_n, z_n)rdr =: \nu_n \rightharpoonup \nu := H^*(w, z)rdr + \alpha_0\delta_0, \tag{3.109}$$

weakly in the sense of measures, where δ_0 is a Dirac mass concentrated at the origin and $\alpha_0 \geqslant 0$.

Recall that

$$\int_0^{+\infty} H^*(w_n, z_n)rdr = 3\mathcal{S}^*(w_n, z_n) \to 3c, \qquad \text{as} \quad n \to +\infty. \tag{3.110}$$

Suppose that the minimizing sequence $(w_n, z_n)_{n\in\mathbb{N}}$ splits into two bumps, one of them centered around the origin and the other one carrying a positive part of the "mass" at infinity (the *dichotomy case* [84]). More precisley, assume that there exist $0 < b < 3c$, and two sequences of radii $r_n, r'_n \to +\infty$, with $\frac{r_n}{r'_n} \to 0$ such that

$$\int_0^{r_n} H^*(w_n, z_n)rdr \to b, \qquad \int_{r_n}^{r'_n} H^*(w_n, z_n)rdr \to 0, \qquad \text{as} \quad n \to +\infty. \tag{3.111}$$

Take a cutoff function $\theta \in C_c^\infty([0,\infty))$, $0 \leqslant \theta \leqslant 1$ such that $\theta \equiv 1$ on [0,1] and $\theta \equiv 0$ on $[2,\infty)$, and define

$$(w_n^1, z_n^1)(r) := \theta\left(\frac{r}{r_n}\right)(w_n, z_n), \qquad (w_n^2, z_n^2) := \left(1 - \theta\left(\frac{r}{r'_n}\right)\right)(w_n, z_n)(r). \tag{3.112}$$

There holds

$$\mathcal{S}^*(w_n, z_n) - \mathcal{S}^*(w_n^1, z_n^1) - \mathcal{S}^*(w_n^2, z_n^2) \to 0, \qquad \text{as} \quad n \to +\infty,$$

and both sequences in (3.112) are Cerami sequences for the functional $\mathcal{S}^*$, that is

$$0 < \mathcal{S}^*(w_n^k, z_n^k) \to c_k < c, \tag{3.113}$$

and

$$\left(1 + \|(w_n^k, z_n^k)\|_{L^{\frac{4}{3}}}\right) d\mathcal{S}^*(w_n^k, z_n^k) \xrightarrow{L^4} 0, \tag{3.114}$$

as $n \to +\infty$, with $k = 1{,}2$.

Remark 3.19. The above estimates can be worked out (along the same lines as in [86, Section 2.1]) recalling that the operator K in (3.95) acts as $\mathcal{D}^{-1}$ and exploiting the decay of the corresponding Green kernel

$$G(x,y) = -\frac{1}{2\pi}\frac{x-y}{|x-y|^2}\cdot,$$

where the dot indicates the Clifford product (see Remark 3.8).

Consider, for instance, the sequence $(w_n^1, z_n^1)_{n\in\mathbb{N}}$. Then the condition (3.114) implies that

$$\langle d\mathcal{S}^*(w_n^1, z_n^1), (w_n^1, z_n^1)\rangle_{L^4\times L^{\frac{4}{3}}} \longrightarrow 0, \qquad \text{as} \quad n \to +\infty, \tag{3.115}$$

that is, the sequence is asymptotically on the Nehari manifold $\mathcal{N}$.

Moreover, there exists a sequence $t_n > 1$ such that $t_n(w_n^1, z_n^1) \in \mathcal{N}, \forall n \in \mathbb{N}$ (see, e.g. [115]). Recalling that H^* is $\frac{4}{3}$-homogeneous, the definition (3.104) of $\mathcal{N}$ then gives

$$\frac{4}{3t_n^{\frac{2}{3}}}\int_0^\infty H^*(w_n^1, z_n^1)rdr = \int_0^\infty \langle K(w_n^1, z_n^1), (w_n^1, z_n^1)\rangle rdr, \qquad \forall n \in \mathbb{N}. \tag{3.116}$$

Combining (3.115) and (3.116) one gets

$$\left(1 - t_n^{-\frac{2}{3}}\right)\frac{4}{3}\int_0^\infty H^*(w_n^1, z_n^1)rdr \longrightarrow 0, \qquad \text{as} \quad n \to +\infty, \tag{3.117}$$

and thus the first condition in (3.111) implies that

$$\lim_{n\to+\infty} t_n = 1. \tag{3.118}$$

Then since $t_n(w_n^1, z_n^1) \in \mathcal{N}$, by (3.111) and (3.118) there holds

$$\mathcal{S}^*(t_n(w_n^2, z_n^2)) = \frac{t_n^{\frac{4}{3}}}{3} \int_0^{+\infty} H^*(w_n^1, z_n^1) r dr \in (0, c),$$

for n large, contradicting the minimality of $c = \inf_{\mathcal{N}} \mathcal{S}^*$. This means that dichotomy cannot occur, and then the sequence of measures $(d\nu_n)_{n\in\mathbb{N}}$ in (3.109) is *tight*. Consequently, up to extraction, (3.110) gives

$$\int_{\mathbb{R}^2} d\nu = 3c. \tag{3.119}$$

Up to suitably rescaling the sequence, we may assume that the weak limit is non-trivial, that is, *vanishing* is also excluded [84]. Indeed, one can find a sequence $\lambda_n > 0, n \in \mathbb{N}$ such that for the rescaled spinor

$$(\tilde{w}_n, \tilde{z}_n)(\cdot) := \lambda_n^{\frac{3}{2}} (w_n, z_n)(\lambda_n \cdot) \tag{3.120}$$

there holds

$$Q_n(1) = \int_0^1 H^*(\tilde{w}_n, \tilde{z}_n) r dr = c, \qquad \forall n \in \mathbb{N}, \tag{3.121}$$

where $Q_n(\cdot)$ is the concentration function of $(\tilde{w}_n, \tilde{z}_n)$ [84, 85].

Assume that $(w, z) = (0,0)$. Then by (3.109) we have $\nu = \alpha_0 \delta_0$, and the normalization (3.121) gives $\alpha_0 \leqslant c$. Then (3.109) and (3.119) imply

$$3c = \int_{\mathbb{R}^2} d\nu = \alpha_0 \leqslant c, \tag{3.122}$$

which is clearly absurd. This allows us to conclude that

$$(w, z) \neq (0,0), \tag{3.123}$$

that is, the above normalization (3.121) rules out the *vanishing case.*

The last step in order to conclude the strong convergence of the minimizing sequence $(w_n, z_n)_{n\in\mathbb{N}}$ is to show that actually $\alpha_0 = 0$ in (3.109). If this is not the case, since by (3.121) there holds $0 < \alpha_0 \leqslant c$, this property and the tightness of the sequence $(d\nu_n)_{n\in\mathbb{N}}$ imply that the sequence $(w_n, z_n)_{n\in\mathbb{N}}$ splits into two parts, one blowing up at the origin, as $n \to +\infty$, and concentrating a portion α_0 of the mass at that point, and another non-trivial part carrying the rest of the mass, essentially localized in an interval of the form

$[1, R]$ (corresponding to an annulus in $\mathbb{R}^2$), for some $R > 0$. Exploiting again the scale-invariance of the problem, one can suitably rescale the sequence, as in (3.120), removing the blowup at the origin, and at the same time "sending at infinity" the bump localized in $[1, R]$. In this way we have created a sequence for which *dichotomy holds* (see (3.111)), and this is not possible, as already shown.

Finally, we conclude that $\alpha_0 = 0$ in (3.109) and then

$$(w_n, z_n) \xrightarrow{L^{\frac{4}{3}}} (w, z) \in \mathcal{N} \qquad \text{as} \quad n \to +\infty. \tag{3.124}$$

Thus $\mathcal{S}^*(w, z) = \min_{\mathcal{N}} \mathcal{S}^*$, and correspondingly

$$(u, v) = (A \circ j^*)\,(w, z),$$

is a critical point of $\mathcal{S}$.

Remark 3.20. Since the Nehari manifold $\mathcal{N}$ contains all critical points of $\mathcal{S}^*$ and $\mathcal{S}^*(w, z) = \min_{\mathcal{N}} \mathcal{S}^*$, we conclude that (w, z) is a *least action* critical point of $\mathcal{S}^*$. In this sense it can be considered a sort of *ground state*. The same remark holds for (u, v), as a critical point of $\mathcal{S}$.

Since we are dealing with a critical equation, smoothness of solutions is not authomatic as standard bootstrap arguments do not apply. Anyway, the regularity result proven in [124] (which holds for weak solutions in L^4) ensures that (u, v) actually is of class C^∞. Being a critical point of $\mathcal{S}$, (u, v) solves the Euler-Lagrange equation (3.35), and smoothness forces

$$u(0) = 0, \tag{3.125}$$

as we cannot have singularities. Moreover, since (u, v) is a non-trivial solution, necessarily

$$v(0) \neq 0. \tag{3.126}$$

Assume, for instance, $v(0) = \lambda > 0$. Since the equation is scale-invariant and odd, as anticipated in Remark (3.7), we get a continuous family of (non-trivial) solutions (u_λ, v_λ) parametrized by $\lambda \neq 0$, applying those symmetries. Uniqueness for (3.35) then allows to conclude the proof.

3.3 Stationary solutions in the massive case

As explained in section 1.2.1, Dirac points for honeycomb Schrödinger operators are protected by the $\mathcal{PT}$ symmetry, and then a mass term may appear in the effective Dirac operator as consequence of a symmetry breaking. In the next section we will quickly show how an effective massive Dirac equation can be derived in that case using the same multiscale expansion as in section 3.2.1. In this case the effective Dirac equation reads as

$$\begin{cases} \partial_t\psi_1 + \overline{\lambda_\#}(\partial_{x_1} + i\partial_{x_2})\psi_2 + im\psi_1 = i(2\beta_2|\psi_1|^2 + \beta_1|\psi_2|^2)\psi_1 \\ \partial_t\psi_2 + \lambda_\#(\partial_{x_1} - i\partial_{x_2})\psi_1 - im\psi_2 = i(\beta_1|\psi_1|^2 + 2\beta_2|\psi_2|^2)\psi_2 \end{cases} \tag{3.127}$$

where $m > 0$ is the mass of the (quasi-)particles described by the equation.

The main result of this section is the existence of exponentially localized smooth solutions to the above equation (3.127), as shown in [26] for a particular case.

Remark 3.21. As remarked in [28], using the main result of [28] one can easily realize that thanks to the asymptotic estimates (3.31) the proof can be easily adapted to the general case (3.127).

In order to agree with the notations adopted in the paper [26] some changes are needed. More precisely, we will exchange spinor components

$$\psi_1 \mapsto \psi_2, \qquad \psi_2 \mapsto \psi_1, \tag{3.128}$$

this does not affect our arguments, but allows us to rewrite the equation in terms of standard Pauli matrices (see chapter 2). Moreover, we will deal with the particular choice of coefficients

$$\beta_1 = 1, \qquad \beta_2 = \frac{1}{2}. \tag{3.129}$$

After these formal manipulations, we obtain the equation

$$i\partial_t\psi + (\mathcal{D} + m\sigma_3)\,\psi = |\psi|^2\psi. \tag{3.130}$$

We look for stationary solutions to the above equations. For a frequency $\omega \in (-m, m)$ in the mass gap of the operator $(\mathcal{D} + m\sigma_3)$ (see section 2.1), we put

$$\psi(t,x) = e^{-it\omega}\psi(x), \qquad (t,x) \in \mathbb{R}_t \times \mathbb{R}^2_x, \tag{3.131}$$

with a little abuse of notation. Then we get the stationary equation

$$(\mathcal{D} + m\sigma_3 - \omega)\,\psi - |\psi|^2\psi = 0. \tag{3.132}$$

Our main result is the following

Theorem 3.22. *(Localized solutions in the massive case, [26, 28]) Equation (3.127) admits a smooth localized solution, with exponential decay at infinity.*

Remark 3.23. For the sake of simplicity we give the proof of Theorem (4.3) for the particular case (3.132).

Remark 3.24. The result presented here is at odds with the case of the pseudo-relativistic operator

$$\sqrt{-\Delta + m^2} \geqslant 0$$

Indeed, a simple Pohozaev-type argument shows that there is no smooth exponentially localized solution to the following equation

$$\left(\sqrt{-\Delta + m^2}\right)\psi - \omega\psi = |\psi|^2\psi \qquad \text{on} \quad \mathbb{R}^2 \tag{3.133}$$

with $0 < \omega < m$. Thus the existence of solutions is related to the presence of the negative part of the spectrum of the Dirac operator.

Weak solutions to (3.132) correspond to critical points of the following functional

$$\mathcal{L}(\psi) := \frac{1}{2}\int \langle (\mathcal{D} + m\sigma_3 - \omega)\,\psi, \psi\rangle - \frac{1}{4}\int |\psi|^4 \tag{3.134}$$

defined for $\psi \in H^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2)$.

The above functional is strongly indefinite, that is, it is unbounded both from above and below, even modulo finite dimensional subspaces. This is due to the unboundedness of $\mathrm{Spec}(\mathcal{D})$. Several techniques have been introduced to deal with such situations (see for instance [114]).

Moreover, the main difficulty in our case is given by the lack of compactness of the Sobolev embedding $H^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2) \hookrightarrow L^4(\mathbb{R}^2, \mathbb{C}^2)$. This implies the failure of some compactness properties used to prove linking results (see [114] and references therein), due to the invariance by translations and scaling.

In what follows we will only give a sketch of the compactness analysis for the above functional, referring to the mentioned papers for more details.

As we will see in the next section, equation (3.132) is compatible with a particular radial ansatz, leading us to work in the closed subspace

$$E = \left\{ \psi \in H^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2) : \psi(r,\vartheta) = \begin{pmatrix} v(r) \\ iu(r)e^{i\vartheta} \end{pmatrix}, u, v : (0, +\infty) \to \mathbb{R} \right\} \tag{3.135}$$

where (r,ϑ) are the polar coordinates of $x \in \mathbb{R}^2$.

Restricting the problem to the subspace E breaks the invariance by translations, and thus to recover compactness one has to deal with the invariance by scaling only. The latter causes the so-called *bubbling phenomenon*, that is, energy concentration associated to the appearance of blow-up profiles. In [72] Isobe analyzed the behavior of a generic Palais-Smale sequence for some critical Dirac equations on compact spin manifolds. The same can be done in our case.

Given a Palais-Smale sequence $(\psi_n) \subseteq H^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2)$ it easy to see that it is bounded, and thus we may suppose, up to extraction, that it weakly converges

$$\psi_n \rightharpoonup \psi_\infty \in H^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2).$$

Generally speaking, the invariance by scaling prevents the strong convergence and we have the profile decomposition

$$\psi_n = \psi_\infty + \sum_{k=1}^{N} \omega_n^k + o(1) \qquad \text{in} \quad H^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2) \tag{3.136}$$

where $N \in \mathbb{N}$ and ω_n^k is a properly rescaled $\mathring{H}^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2)$-solution of the limit equation

$$\mathcal{D}\varphi = |\varphi|^2\varphi$$

centered around points $a_n^k \to a^k \in \mathbb{R}^2$, as $n \to +\infty$, for $1 \leqslant k \leqslant N$.

The *bubbles* ω_n^k are in a finite number, since one can prove a uniform lower bound for their energy. Moreover, this implies that we have compactness only in a suitable energy range and gives a treshold value for the appearance of bubbles in min-max methods (see [114]). Then there holds

$$|\psi_n|^4 dx \rightharpoonup |\psi_\infty|^4 dx + \sum_{k=1}^{N} \nu_k \delta_{a^k}, \tag{3.137}$$

weakly in the sense of measures.Here $\nu_k \geqslant 0$ and the δ_{a^k} are delta measures concentrated at a^k. Morever, since we are essentially working with radial functions, it's not hard to see that the blow-up can only occur at the origin, that is, we actually have

$$|\psi_n|^4 dx \rightharpoonup |\psi_\infty|^4 dx + \nu\delta_0 \tag{3.138}$$

with $\nu \geqslant 0$ and δ_0 being the delta concentrated at the origin.

We thus conclude that in order to recover compactness for the variational problem one should be able to control the behavior of Palais-Smale sequences near the origin.

However, our proof is based on a shooting method and thus not variational. In this case the concentration phenomenon (3.138) manifests itself in the difficulty of controlling the behavior of solutions of the resulting dynamical system when initial data are large. This makes the analysis quite delicate and requires a careful asymptotic expansion of the solution, after a suitable rescaling (see section 3.3.3).

We mention that the first rigorous existence result of stationary solutions for the Dirac equation via shooting methods is due to Cazenave and Vazquez [40], who studied the Soler model for elementary fermions. Subsequently, those methods have been used to prove the existence of excited states [17] for the Soler model and in mean field theories for nucleons (see e.g. [53],[81], [52] and references therein). We remark that a variational proof has been given by Esteban and Séré in [54], under fairly general assumptions on the self-interaction. In particular, after a suitable radial ansatz, they prove a multiplicity result exploiting the Lorentz-invariance. Remarkably, their method works without any growth assumption on the nonlinearity. However, the proof is designed to deal with the Lorentz-invariant form of the nonlinear term and is not applicable in our case. In [44] Ding and Wei proved an existence result for the 3D Dirac equation with a subcritical Kerr-type interaction. The case of a critical nonlinearity in 3D has been investigated by Ding and Ruf [43] in the semiclassical regime, using variational techniques. They take advantage of the presence of a negative potential to prove compactness properties. However, in our case we deal with a critical Kerr nonlinearity without additional assumptions and so we need to adopt a different strategy.

3.3.1 Formal derivation

The aim of this section is to derive the massive Dirac equation (3.127) thanks to a multiscale expansion as in section 3.2.1. We adopt the same notations here.

As already remarked, breaking the $\mathcal{PT}$ symmetry lifts the conical degeneracy in the dispersion relation of a honeycomb Schrödinger operator $(-\Delta + V)$ admitting Dirac points. Let us consider the following equation

$$(-\Delta + V + \varepsilon W - \mu_*)\, u = |u|^2 u, \tag{3.139}$$

that is, we consider a potential perturbation of (3.9) where we add a linear term W breaking parity. More precisely, we assume that W is *odd*

$$W(-x) = -W(x), \qquad \forall x \in \mathbb{R}^2. \tag{3.140}$$

The only difference with respect to the analysis outlined in section 3.2.1 is an additional term at order $\mathcal{O}(\varepsilon)$ corresponding to the potential εW in (3.139). Then we have to compute the projections

$$\langle WU_0, \Phi_k\rangle_{L^2(\Omega)} = \sum_{j=1}^{2} \psi_j \langle W\Phi_j, \Phi_k\rangle_{L^2(\Omega)}, \qquad k = 1{,}2. \tag{3.141}$$

Recall that

$$\Phi_2(x) = \overline{\Phi_1(-x)}, \tag{3.142}$$

and this relation allows us to compute

$$\begin{aligned} \langle W\Phi_2, \Phi_1\rangle_{L^2(\Omega)} &= \int_\Omega (W\Phi_2)(x)\overline{\Phi_1(x)}dx = \int_\Omega W(x)\overline{\Phi_1(-x)\Phi_1(x)}dx \\ &=^{y=-x} \int_{-\Omega} W(-y)\overline{\Phi_1(y)\Phi_1(-y)}dy = -\int_\Omega (W\Phi_2)(y)\overline{\Phi_1(y)}dy \\ &= -\langle W\Phi_2, \Phi_1\rangle_{L^2(\Omega)}, \end{aligned} \tag{3.143}$$

where we have also used (3.140). We thus obtain

$$\langle W\Phi_2, \Phi_1\rangle_{L^2(\Omega)} = \langle W\Phi_1, \Phi_2\rangle_{L^2(\Omega)} = 0. \tag{3.144}$$

Moreover, arguing as in (3.143) one easily finds

$$\langle W\Phi_1, \Phi_1\rangle_{L^2(\Omega)} = -\langle W\Phi_2, \Phi_2\rangle_{L^2(\Omega)}. \tag{3.145}$$

and then

$$\begin{aligned} \sum_{j=1}^{2} \psi_j \langle W\Phi_j, \Phi_1\rangle_{L^2(\Omega)} &= \langle W\Phi_1, \Phi_1\rangle_{L^2(\Omega)} \\ \sum_{j=1}^{2} \psi_j \langle W\Phi_j, \Phi_k\rangle_{L^2(\Omega)} &= -\langle W\Phi_1, \Phi_1\rangle_{L^2(\Omega)}. \end{aligned} \tag{3.146}$$

Assuming that $m := \langle W\Phi_1, \Phi_1\rangle_{L^2(\Omega)} > 0$, we obtain the mass term in (3.127).

3.3.2 Existence by shooting method

To begin with, we first convert equation (3.132) into a dynamical system thanks to a particular ansatz. Then we will give some qualitative properties of the flow, particularly useful in understanding the long-time behavior of the system.

Passing to polar coordinates in $\mathbb{R}^2$ $(x,y) \mapsto (r,\vartheta)$, the equation

$$(\mathcal{D} + m\sigma_3 - \omega)\,\psi - |\psi|^2\psi = 0$$

reads as

$$\begin{cases} -e^{-i\vartheta}\left(i\partial_r + \dfrac{\partial_\vartheta}{r}\right)\psi_2 = \left(|\psi_1|^2 + |\psi_2|^2\right)\psi_1 - (m-\omega)\psi_1, \\ \;\; -e^{i\vartheta}\left(i\partial_r - \dfrac{\partial_\vartheta}{r}\right)\psi_1 = -\left(|\psi_1|^2 + |\psi_2|^2\right)\psi_2 - (m+\omega)\psi_2. \end{cases} \tag{3.147}$$

where $\psi = \begin{pmatrix}\psi_1 \\ \psi_2\end{pmatrix} \in \mathbb{C}^2$, and this suggests the following ansatz (see [41]):

$$\psi(r,\vartheta) = \begin{pmatrix} v(r)e^{iS\vartheta} \\ iu(r)e^{i(S+1)\vartheta} \end{pmatrix} \tag{3.148}$$

with u and v real-valued and $S \in \mathbb{Z}$. In the sequel, we set $S = 0$.

Plugging the above ansatz into the equation one gets

$$\begin{cases} \dot{u} + \dfrac{u}{r} = (u^2+v^2)v - (m-\omega)v \\ \qquad \dot{v} = -(u^2+v^2)u - (m+\omega)u \end{cases} \tag{3.149}$$

Thus we are lead to study the flow of the above system.

In particular, since we are looking for localized states, we are interested in solutions to (3.149) such that

$$(u(r), v(r)) \to (0{,}0) \qquad \text{as} \qquad r \to +\infty$$

In order to avoid singularities and to get non-trivial solutions, we choose as initial conditions

$$u(0) = 0 \quad , \quad v(0) = \lambda \neq 0$$

Moreover, the symmetry of the system allows us to consider only the case $\lambda > 0$.

Studying the long-time behavior of the flow of (3.149) it is useful to introduce the following system

$$\begin{cases} \dot{u} = (u^2+v^2)v - (m-\omega)v \\ \dot{v} = -(u^2+v^2)u - (m+\omega)u \end{cases} \tag{3.150}$$

Heuristically, (3.149) should reduce to (3.150) in the limit $r \to +\infty$ (u being bounded), that is, dropping the singular term in the first equation.

As one can easily check, (3.150) is the hamiltonian system associated with the function

$$H(u,v) = \frac{(u^2+v^2)^2}{4} + \frac{m}{2}(u^2-v^2) + \frac{\omega}{2}(u^2+v^2) \tag{3.151}$$

It is easy to see that the level sets of the hamiltonian

$$\{H(u,v) = c\}$$

are compact, for all $c \in \mathbb{R}$, so that the flow is globally defined.

The equilibria of the hamiltonian flow are the points

$$(0{,}0), (0, \pm\sqrt{m-\omega}) \tag{3.152}$$

and there holds

$$H(0{,}0) = 0, \quad H(0, \pm\sqrt{m-\omega}) < 0 \tag{3.153}$$

Local existence and uniqueness of solutions of (3.149) are guaranteed by the following

Lemma 3.25. *Let* $\lambda > 0$. *There exist* $0 < R_\lambda \leqslant +\infty$ *and* $(u,v) \in C^1([0,R_\lambda),\mathbb{R}^2)$ *unique maximal solution to (3.149), which depends continuously on* λ *and uniformly on* $[0,R]$ *for any* $0 < R < R_\lambda$.

Proof. We can rewrite the system in integral form as

$$\begin{cases} u(r) = \dfrac{1}{r}\displaystyle\int_0^r sv(s)[u^2(s)+v^2(s)-(m-\omega)]ds \\ v(r) = \lambda - \displaystyle\int_0^r u(s)[(u^2(s)+v^2(s)) + (m+\omega)]ds \end{cases} \tag{3.154}$$

where the r.h.s. is a Lipschitz continuous function. Then the claim follows by a contraction mapping argument, as in [40]. □

Given $\lambda > 0$, define

$$H_\lambda(r) := H(u_\lambda(r), v_\lambda(r)) \quad , \quad r \in [0, R_\lambda) \tag{3.155}$$

where (u_λ, v_λ) is the solution of (3.149) such that $(u(0), v(0)) = (0, \lambda)$.

A simple computation gives

$$\dot{H}_\lambda(r) = -\frac{u_\lambda^2}{r}(m + \omega + u_\lambda^2(r) + v_\lambda^2(r)) \leqslant 0 \quad , \quad \forall r \in [0, R_\lambda) \tag{3.156}$$

so that the energy H is non-increasing along the solutions of (3.149).

This implies that $\forall r \in [0, R_x)$, $(u_\lambda(r), v_\lambda(r)) \in \{H(u, v) \leqslant H(0, \lambda)\}$, the latter being a compact set. Thus there holds

Lemma 3.26. *Every solution to (3.149) is global.*

Remark 3.27. The above result is in contrast with the case of Lorentz-invariant models in 3D ([17]), where the energy has no definite sign and blow-up may occur.

The following lemma indeed shows that the solutions to (3.149) are close to the hamiltonian flow (3.150) as $r \to +\infty$. The proof is the same as the one given in [40].

Lemma 3.28. *Let (f, g) be the solution of (3.150) with initial data (f_0, g_0). Let $(u_n^0, v0_n)$ and ρ_n be such that*

$$\rho_n \xrightarrow{n \to +\infty} +\infty \qquad \textit{and} \qquad (u_n, v_n) \xrightarrow{n \to +\infty} (f_0, g_0)$$

Consider the solution of

$$\begin{cases} \dot{u}_n + \dfrac{u_n}{r + \rho_n} = (u_n^2 + v_n^2)v_n - (m - \omega)v_n \\ \qquad\qquad \dot{v}_n = -(u_n^2 + v_n^2)u_n - (m + \omega)u_n \end{cases}$$

such that $u_n(0) = u_n^0$ and $v_n(0) = v_n^0$.

Then (u_n, v_n) converges to (f, g) uniformly on bounded intervals.

Since we know from (3.156) that the energy H_λ decreases along the flow of (3.149) and that each solution is bounded, Lemma (3.28) allows us to conclude (see the proof of Lemma (3.31)) that any solution must tend to an equilibrium of the hamiltonian flow (3.150). Thus a solution eventually entering the negative energy region

$$\{H(u, v) < 0\}$$

will converge to

$$(0, \pm\sqrt{m-\omega})$$

spiraling toward that point. A proof of this property follows along the same lines of the analogous one given in [53]. This is illustrated by the following picture:

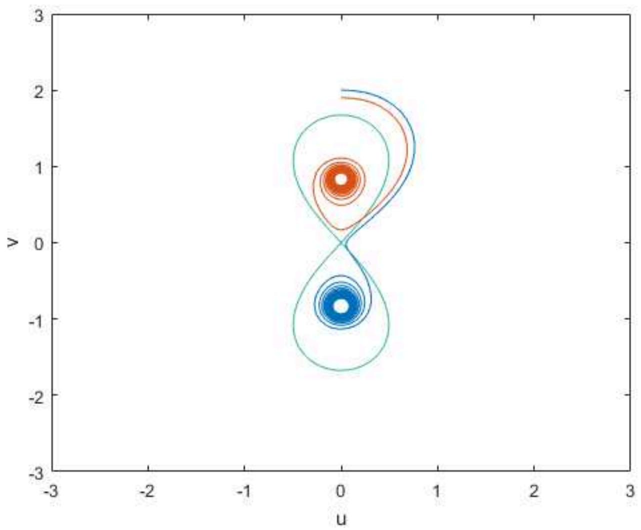

Figure 3.2. The energy level $\{H = 0\}$ and two solutions entering the negative energy set $\{H < 0\}$.

If, on the contrary, there holds

$$H_\lambda(r) > 0, \qquad \forall r > 0$$

then necessarily the solution tends to the origin, thus corresponding to a localized solution of our PDE.

In our proof we use some ideas from [81], [91].

Definition 3.29. Put $I_{-1} = \emptyset$. For $k \in \mathbb{N}$ we define

(3.157)
$$A_k = \left\{\lambda > 0 : \lim_{r\to+\infty} H_\lambda(r) < 0, v_\lambda \text{ changes sign } k \text{ times on } (0,+\infty)\right\}$$
$$I_k = \left\{\lambda > 0 : \lim_{r\to+\infty} (u_\lambda(r), v_\lambda(r)) = (0,0), v_\lambda \text{ changes sign } k \text{ times on } (0,+\infty)\right\}.$$

It is immediate so see that

$$A_0 \neq \emptyset$$

as it includes the interval $\left(0, \sqrt{2(m-\omega}\right]$, since

$$\{0\} \times \left(0, \sqrt{2(m-\omega)}\right] \subseteq \{(u,v) \in \mathbb{R}^2 : H(u,v) \leqslant 0\}$$

Moreover, numerical simulations indicate that the set A_0 is bounded and that A_1 is non-empty and unbounded. This implies that I_0 is non empty (see 3.33). Solutions tending to the origin are expected to appear in the shooting procedure when λ passes from A_k to A_{k+1}, as in (Figure 3.2).

Remark 3.30. We found no numerical evidence for the existence of excited states. This may lead to conjecture that there are no nodal solutions, that is $I_k = \emptyset$ for $k > 1$. The absence of excited states is compatible with the bubbling phenomenon (see the previous section), which might prevent the existence of those solutions. However in 3D Lorentz-invariant models ([52],[17]) it is known that they exist.

In this section we show that I_0 is non empty, thus proving (Theorem 4.3). This will be achieved in several intermediate steps.

We start with some preliminary lemmas, which are an adaptation of analogous results from [81].

Lemma 3.31. *Let (u_λ, v_λ) be a solution of (3.149) such that v_λ changes sign a finite number of times and*

$$\lim_{r\to+\infty} H_\lambda(r) \geqslant 0$$

then

$$|u_\lambda(r)| + |v_\lambda(r)| \leqslant Ce^{-\left(\frac{m-\omega}{2}\right)r} \quad , \quad \forall r \geqslant 0 \tag{3.158}$$

and thus

$$\lim_{r\to+\infty} (u_\lambda(r), v_\lambda(r)) = (0{,}0)$$

Proof. We start by showing that under the above assumptions there exists $\overline{R} \in (0, +\infty)$ such that

$$u_\lambda(r)v_\lambda(r) > 0 \quad , \quad \forall r \geqslant \overline{R} \tag{3.159}$$

Since v_λ changes sign a finite number of times, we may suppose w.l.o.g. that for some $R > 0$

$$v_\lambda(r) > 0 \quad , \quad \forall r \geqslant R$$

We have to prove that $\exists R < \overline{R} < +\infty$ such that

$$u_\lambda(r) > 0 \quad , \quad \forall r \geqslant \overline{R}$$

Assume, by contradiction, that

$$u_\lambda(r) < 0 \quad , \quad \forall r > R$$

Then the second equation of (3.149) implies that $\dot{v}_\lambda(r) > 0, \forall r > R$, and v_λ is increasing for $r > R$. Thus

$$\lim_{r \to +\infty} v_\lambda(r) = \delta \in (0, +\infty]$$

Indeed, we cannot have $\delta = +\infty$ as in that case

$$\lim_{r \to +\infty} H_\lambda(r) = +\infty$$

contradicting the fact that H_λ is decreasing along solutions of (3.149).

Let $(\rho_n)_n \subseteq \mathbb{R}$ be a sequence such that

$$\lim_{n \to +\infty} \rho_n = +\infty \quad , \quad \lim_{n \to +\infty} u_x(\rho_n) = \lambda$$

for some $\lambda \in \mathbb{R}$, and consider the solution (U, V) of (3.150) such that

$$(U(0), V(0)) = (\lambda, \delta)$$

By (3.28), it follows that $(u_\lambda(\rho_n + *), v_\lambda(\rho_n + *))$ converges uniformly to (U, V) on bounded intervals. Since

$$\lim_{n \to +\infty} v_\lambda(\rho_n + r) = \delta \quad , \quad \forall r > 0$$

we have $V(r) = \delta$, for any $r \geqslant 0$. The second equation of (3.150) implies that $U(r) = 0$ for all $r > 0$.

We conclude that (U, V) is an equilibrium of the hamiltonian flow (3.150). Since $\delta > 0$,

$$(\lambda, \delta) = (0, \sqrt{m - \omega})$$

This is absurd, since we would have

$$0 \leqslant \lim_{r \to +\infty} H_\lambda(r) \leqslant H\left(0, \sqrt{m - \omega}\right) < 0$$

Thus there exists $\overline{R} \in (R, +\infty)$ such that $u_\lambda(\overline{R}) = 0$. Note that we have

$$\dot{u}_\lambda(\overline{R}) > 0$$

Indeed, $\dot{u}_\lambda(\overline{R}) = v_x(\overline{R})\left[v_\lambda^2(\overline{R}) - (m-\omega)\right] > 0$ where the term in the r.h.s. is positive, otherwise the point $(0, v_\lambda(\overline{R}))$ would belong to the negative energy region, contradicting our assumptions on $H_\lambda(r)$.

Now suppose that there exists $R < \overline{R} < R'$ such that $u_\lambda(R') = 0$ and $u_\lambda(r) > 0$ on $(\overline{R}, R')$. This implies that $\dot{u}_\lambda$ is negative in a left neighborhood of R'. By the first equation of (3.149), we get

$$v_\lambda^2(R') - (m-\omega) \leqslant 0$$

Then $(0, v_\lambda(R')) \in \{H(u,v) < 0\}$, and this is absurd as already remarked.

We thus conclude that

$$u_\lambda(r) > 0 \quad , \quad \forall r \geqslant \overline{R} \tag{3.160}$$

The second equation of (3.149) shows that v_λ is decreasing on $(\overline{R}, +\infty)$ and by (3.28), arguing as above, it can be proved that

$$\lim_{r\to+\infty}(u_\lambda(r), v_\lambda(r)) = (0,0) \tag{3.161}$$

We now prove the exponential decay.

By (3.149), (5.49), (3.160), we have for all $r > \overline{R}$

$$\begin{cases} \dot{u}_\lambda \leqslant \dfrac{(m-\omega)}{2} v_\lambda - (m-\omega) v_x \\ \dot{v} \leqslant -(m+\omega) u_\lambda \end{cases} \tag{3.162}$$

Then

$$\frac{d}{dr}(u_\lambda + v_\lambda) \leqslant -\frac{(m-\omega)}{2}(u_\lambda + v_\lambda)$$

for all $r > \overline{R}$. Then the claim follows, since

$$u_\lambda(r), v_\lambda(r) > 0, \quad \forall r \geqslant \overline{R}.$$

□

Lemma 3.32. *There exists a constant $C_0 > 0$ such that, if for some $R > 1$*

1. $H_\lambda(R) < \frac{C_0}{R}$;

2. $u_\lambda(R)v_\lambda(R) > 0$ *and* $v_\lambda^2(R) < 2(m-\omega)$;

3. v_λ *changes sign* k *times on* $[0,R]$;

then $\lambda \in A_k \cup I_k \cup A_{k+1}$.

Proof. Suppose, by contradiction, that $\lambda \notin A_k \cup I_k \cup A_{k+1}$.

W.l.o.g. we can assume that $u_\lambda(R) > 0$ and $v_\lambda(R) > 0$. Let

$$\overline{R} := \inf\{r > R \ : \ u_\lambda(r) \leqslant 0\} \in (R, +\infty]$$

Note that v_λ changes sign exactly once in $(R, \overline{R})$. Indeed, as long as $u_\lambda > 0$ the second equation of (3.149) shows that v_λ is decreasing. Moreover we cannot have $v_\lambda(r) > 0$ for all $(R, \overline{R})$, as in that case the solution would enter the negative energy zone or tend to the origin. This is impossible, since $\lambda \notin A_k \cup I_k$.

Now suppose that $\overline{R} = +\infty$. We have seen that there exists $R < \tilde{R} < +\infty$ such that $v_\lambda < 0$ on $(\tilde{R}, \overline{R})$. Arguing as in the proof of (Lemma 3.31), one easily sees that

$$\lim_{r\to+\infty} v_\lambda(r) = \delta \in (-\infty, 0)$$

Moreover, the solution tends to an equilibrium (λ, δ) of the hamiltonian system (3.150), as $r \longrightarrow +\infty$.

Thus $(\lambda, \delta) = (0, -\sqrt{m-\omega})$, giving a contradiction as

$$0 \leqslant \lim_{r\to+\infty} H_\lambda(r) = H\left(0, -\sqrt{(m-\omega)}\right) < 0$$

Then $\overline{R} < +\infty$ and we have

$$u_\lambda(\overline{R}) = 0 \qquad , \qquad v_\lambda(\overline{R}) \leqslant -\sqrt{2(m-\omega)}$$

since we must have $H_\lambda(\overline{R}) > 0$.

Let $R < R_1 < R_2 < \overline{R}$ be such that

$$v_\lambda(R_1) = -\frac{\sqrt{m-\omega}}{2} \quad , \quad v_\lambda(R_2) = -\sqrt{m-\omega} \tag{3.163}$$

Since $R > 1$, we have $H_\lambda(R) < C_0$ and if C_0 is sufficiently small we have that

$$u_\lambda(r) \leqslant \sqrt{m-\omega} \quad , \quad \forall r \in [R_1, R_2] \tag{3.164}$$

We have, since v_λ is decreasing and by (3.149,3.178,3.163)

$$\frac{\sqrt{m-\omega}}{2} = v_\lambda(R_1) - v_\lambda(R_2) = -\int_{R_1}^{R_2} \dot{v}_\lambda(r)dr = \int_{R_1}^{R_2} \sqrt{m-\omega}\,(3m-\omega)\,dr$$

and then

$$(R_2 - R_1) \geqslant \frac{1}{2(3m-\omega)} \tag{3.165}$$

Moreover, a simple computation gives

$$\frac{1}{r}\frac{d}{dr}\Big(r^2 H_\lambda(r)\Big) = 2H_\lambda(r) + r\dot{H}_\lambda(r) = -\frac{u_\lambda^4(r)}{2} + \frac{v_\lambda^2(r)}{2}\Big[v_\lambda^2(r) - 2(m-\omega)\Big] \tag{3.166}$$

and then

$$\frac{d}{dr}\Big(r^2 H_\lambda(r)\Big) < 0 \quad , \quad \forall r \in [R, R_2] \tag{3.167}$$

By (3.163,3.166) we have

$$\begin{aligned} (R_2)^2 H_\lambda(R_2) - (R_1)^2 H_\lambda(R_1) &\leqslant -\int_{R_1}^{R_2} \frac{(m-\omega)^2}{2} r dr \\ &= -\frac{(m-\omega)^2}{4}(R_2+R_1)(R_2-R_1) \\ &\leqslant -\frac{(m-\omega)^2}{4(3m-\omega)} R \end{aligned} \tag{3.168}$$

Since the map $r \mapsto r^2 H_\lambda(r)$ is decreasing on $[R, R_2]$ by (3.167), then (3.168) implies that

$$\begin{aligned} (R_2)^2 H_\lambda(R_2) &\leqslant (R_1)^2 H_\lambda(R_1) - \frac{(m-\omega)^2}{4(3m-\omega)} R \\ &\leqslant R^2 \left(H_\lambda(R) - \frac{(m-\omega)^2}{4R(3m-\omega)} \right) \leqslant 0 \end{aligned} \tag{3.169}$$

if $C_0 \leqslant \frac{(m-\omega)^2}{4(3m-\omega)}$. Then

$$H_\lambda(R_2) \leqslant 0$$

reaching a contradiction, and the lemma is proved. □

The next lemma gives the main properties of the sets A_k and I_k.

Lemma 3.33. *For all $k \in \mathbb{N}$ we have*

1. *A_k is an open set;*

2. *if* $\lambda \in I_k$ *then there exists* $\varepsilon > 0$ *such that* $(\lambda - \varepsilon, \lambda + \varepsilon) \subseteq A_k \cup I_k \cup A_{k+1}$*;*

3. *if* $A_k \neq \emptyset$ *and it is bounded, we have* $\sup A_k \in I_k$*;*

4. *if* $I_k \neq \emptyset$ *and it is bounded, then* $\sup I_k \in I_k$*.*

Proof. 1. It follows from the continuity of the flow (3.149) w.r.t. the initial datum (Lemma 3.25);

2. Let $\lambda \in I_k$. By Lemma (3.31)

$$|u_\lambda(r)| + |v_\lambda(r)| \leqslant C \exp\left(-\frac{m-\omega}{2} r\right) \quad , \quad \forall r \geqslant 0$$

and then, given $C_0 > 0$ as in Lemma (3.166), $\exists R > 1$ such that $H_\lambda(R) < \frac{C_0}{R}$, $u_\lambda(R) v_\lambda(R) > 0$ and v_λ changes sign k times on $[0, R]$.

The continuity of the flow (3.149) implies that the same holds for an initial datum $y \in (\lambda - \varepsilon, \lambda + \varepsilon)$ for $\varepsilon > 0$ small. The claim then follows by Lemma (3.166).

3. Let $\lambda = \sup A_k$ and $(\lambda_i) \subseteq A_k$ such that $\lim_{i \to +\infty} \lambda_i = \lambda$.

If we suppose that $\lambda \in A_r$ for some $r \in \mathbb{N}$, then by continuity of the flow we also have $\lambda_i \in A_r$, for i large. This implies that $r = k$, that is, $\lambda \in A_k$ which is absurd because A_k is an open set, by point (1).

Thus there holds $\lambda \in I_s$, for some $s \in \mathbb{N}$, and by point (2) there exists $\varepsilon > 0$ such that

$$\lambda \in A_s \cup I_s \cup A_{s+1}$$

which implies that the same holds for λ_i, provided i is large. Then, as before, we have $s = k$.

Moreover, as already remarked

$$\lambda \notin \bigcup_{j \in \mathbb{N}} A_j$$

and then the claim follows.

4. Arguing as in the proof of point (3) we get that

$$\sup I_k \in I_r$$

for some $r \in \mathbb{N}$. Then we conclude as before, using point (2).

□

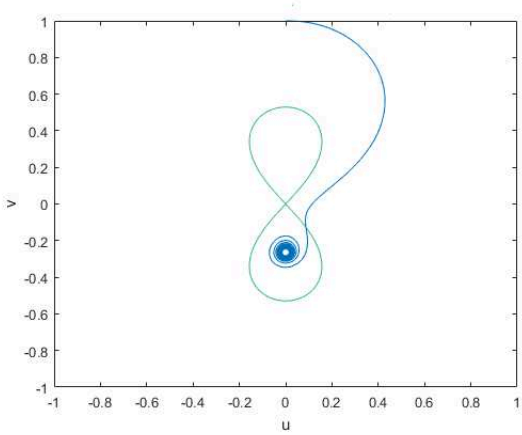

Figure 3.3. A solution entering the lower half-plane $\{v < 0\}$.

We want to prove that the set A_0 is bounded, showing that if $\lambda > 0$ is large enough then there exists $R_\lambda > 0$ such that $v_\lambda(R_\lambda) = 0$, as strongly suggested by numerical simulations (see Figure 3.3.2). To do so we relate solutions corresponding to such data to those of a limiting problem, inspired by [91].

3.3.3 Asymptotic expansion

In this section we provide, after a suitable scaling, a precise asymptotic expansion that will allow us to control the behavior of the solution in term of the initial datum.

Put $\varepsilon = \lambda^{-1}$ and consider the following rescaling

$$\begin{cases} U_\varepsilon(r) = \varepsilon u_\lambda(\varepsilon^2 r) \\ V_\varepsilon(r) = \varepsilon v_\lambda(\varepsilon^2 r) \end{cases} \tag{3.170}$$

Using (3.149) we find the system for $(U_\varepsilon, V_\varepsilon)$:

$$\begin{cases} \dot{U}_\varepsilon + \dfrac{U_\varepsilon}{r} = (U_\varepsilon^2 + V_\varepsilon^2)V_\varepsilon - \varepsilon^2(m-\omega)V_\varepsilon \\ \dot{V}_\varepsilon = -(U_\varepsilon^2 + V_\varepsilon^2)U_\varepsilon - \varepsilon^2(m+\omega)U_\varepsilon \end{cases} \tag{3.171}$$

together with the initial conditions $U_\varepsilon(0) = 0$, $V_\varepsilon(0) = 1$.

The limiting problem as $\varepsilon \to 0$ (and thus $\lambda \to +\infty$) is

$$
\begin{cases} \dot{U}_0 + \dfrac{U_0}{r} = (U_0^2 + V_0^2)V_0 \\ \dot{V}_0 = -(U_0^2 + V_0^2)U_0 \end{cases} \tag{3.172}
$$

with $U_0(0) = 0$, $V_0(0) = 1$.

As in [15] we consider the family of spinors given by

$$
\varphi(y) = f(y)(1 - y) \cdot \varphi_0 \qquad y \in \mathbb{R}^2 \tag{3.173}
$$

where $\varphi_0 \in \mathbb{C}^2$, $f(y) = \frac{2}{1+|y|^2}$ and the dot represents the Clifford product.

It can be easily checked that they are $\mathring{H}^{\frac{1}{2}}(\mathbb{R}^2, \mathbb{C}^2)$-solutions to the following Dirac equation

$$
\mathcal{D}\varphi = |\varphi|^2\varphi \tag{3.174}
$$

Remark 3.34. The spin structure of euclidean spaces is quite explicit and the spinors given in (5.44) can be rewritten in matrix notation, as

$$
\varphi(y) = f(y)(1_2 + iy_1\sigma_1 + iy_2\sigma_2) \cdot \varphi_0 \qquad y \in \mathbb{R}^2
$$

1_2 and σ_i being the identity and the Pauli matrices, respectively.

See [73] for more details.

A straightforward (but tedious) computation shows that the spinors defined in (5.44) are of the form of the ansatz (3.148), thus being solutions to the system (3.172). Exploiting the conformal invariance of (3.174) (see [72]) one can easily see that the solution matching the above initial conditions is

$$
\left(U_0(r) = \frac{2r}{4 + r^2}, V_0(r) = \frac{4}{4 + r^2} \right) \tag{3.175}
$$

Lemma 3.35. *We have*

$$
(U_\varepsilon, V_\varepsilon) \xrightarrow{\varepsilon \to 0} (U_0, V_0)
$$

uniformly on $[0, T]$*, for all* $T > 0$*, where* (U_0, V_0) *is the solutions to the limiting problem (3.172).*

Proof. Fix $T > 0$ and let $r \in [0, T]$.

Remark that the system (3.171) is equivalent to

$$\begin{cases} U_\varepsilon(r) = \dfrac{1}{r}\displaystyle\int_0^r sV_\varepsilon(s)[U_\varepsilon^2(s) + V_\varepsilon^2(s) - \varepsilon^2(m-\omega)]ds \\ V_\varepsilon(r) = 1 - \displaystyle\int_0^r U_\varepsilon(s)[(U_\varepsilon^2(s) + V_\varepsilon^2(s)) + \varepsilon^2(m+\omega)]ds \end{cases} \tag{3.176}$$

Similarly, we can rewrite (3.172) as

$$\begin{cases} U_0(r) = \dfrac{1}{r}\displaystyle\int_0^r sV_0(s)(U_0^2(s) + V_\varepsilon^2(s))ds \\ V_0(r) = 1 - \displaystyle\int_0^r U_0(s)(U_0^2(s) + V_0^2(s))ds \end{cases} \tag{3.177}$$

Arguing as for (3.149), for each fixed $\varepsilon > 0$ we associate a hamiltonian to the system (3.171)

$$\tilde{H}_\varepsilon(U,V) := \frac{(U^2+V^2)^2}{4} + \varepsilon^2\frac{m}{2}(U^2 - V^2) + \varepsilon^2\frac{\omega}{2}(U^2+V^2)$$

It's easy to see that $\tilde{H}_\varepsilon$ is decreasing along the flow, so that

$$\tilde{H}_\varepsilon(U_\varepsilon(r), V_\varepsilon(r)) \leqslant \tilde{H}_\varepsilon(0,1) \leqslant 1 \qquad \forall r \geqslant 0.$$

The coercivity of H_ε then implies that

$$|U_\varepsilon(r)| + |V_\varepsilon(r)| \leqslant C \qquad \forall r \geqslant 0 \tag{3.178}$$

for some $C > 0$ independent of ε.

By (3.176,3.177) and since $r \in [0,T]$ we get

$$\begin{aligned} |U_\varepsilon(r) - U_0(r)| + |V_\varepsilon(r) - V_0(r)| \leqslant & \int_0^r \left| V_\varepsilon(V_\varepsilon^2 + U_\varepsilon^2) - V_0(V_0^2 + U_0^2)\right| ds \\ & + \int_0^r \left| U_\varepsilon(V_\varepsilon^2 + U_\varepsilon^2) - U_0(V_0^2 + U_0^2)\right| ds + 2\varepsilon^2 mT \end{aligned} \tag{3.179}$$

It is not hard to see that the first two integrands in the r.h.s of the above inequality are locally Lipschitz. Then by (3.178) we have

$$|U_\varepsilon(r) - U_0(r)| + |V_\varepsilon(r) - V_0(r)| \lesssim \int_0^r (|U_\varepsilon - U_0| + |V_\varepsilon - V_0|)\, ds + 2\varepsilon^2 mT \tag{3.180}$$

Since $r \in [0,T]$, the Gronwall lemma gives

$$|U_\varepsilon(r) - U_0(r)| + |V_\varepsilon(r) - V_0(r)| \lesssim \varepsilon^2 \tag{3.181}$$

thus proving the claim. □

The above results is not enough to conclude that V_ε changes sign, since $V_0 > 0$ for all $r \geqslant 0$.

We obtain a more refined analysis of the behavior of the solution thanks to a continuity argument.

We consider the solution $(U_\varepsilon, V_\varepsilon)$ as a perturbation of (U_0, V_0), as follows:

$$\begin{cases} U_\varepsilon(r) = U_0(r) + \varepsilon^2 h_1(r) + \varepsilon^4 h_2(r,\varepsilon) \\ V_\varepsilon(r) = V_0(r) + \varepsilon^2 k_1(r) + \varepsilon^4 k_2(r,\varepsilon) \end{cases} \tag{3.182}$$

and substituting into (3.171) we get the following linear system for ε^2-order terms

$$\begin{cases} \dot{h}_1 + \dfrac{h_1}{r} = -(m-\omega)V_0 + 2U_0V_0h_1 + (U_0^2 + 3V_0^2)k_1 \\ \dot{k}_1 = -(m+\omega)U_0 - 2U_0V_0k_1 - (3U_0^2 + V_0^2)h_1 \end{cases} \tag{3.183}$$

and we impose the initial conditions

$$h_1(0) = 0 \qquad , \quad k_1(0) = 0 \tag{3.184}$$

Rewriting (3.183) in integral form, as in (3.154), we have:

$$\begin{cases} |h_1(r)| \leqslant \displaystyle\int_0^r (m-\omega)V_0 ds + \int_0^r \Big[2U_0V_0|h_1| + (U_0^2 + 3V_0^2)|k_1|\Big]\, ds \\ |k_1(r)| \leqslant \displaystyle\int_0^r (m+\omega)U_0 ds + \int_0^r \Big[2U_0V_0|k_1| + (3U_0^2 + V_0^2)|h_1|\Big]\, ds \end{cases} \tag{3.185}$$

Remark that

$$U_0V_0(r) + V_0^2(r) \leqslant U_0^2(r) \leqslant V_0 \quad , \quad \forall r > 2$$

and that

$$V_0 \in L^1(\mathbb{R}^+).$$

Moreover, there holds

$$U_0(r) = \frac{2r}{4+r^2} \sim \frac{2}{r} \qquad \text{as} \quad r \longrightarrow +\infty. \tag{3.186}$$

Then summing up both sides of (3.185) we get:

$$|h_1(r)| + |k_1(r)| \lesssim \int_0^r U_0 ds + \int_0^r (|h_1| + |k_1|)\, V_0 ds \tag{3.187}$$

The Gronwall inequality thus gives:

$$|h_1(r)| + |k_1(r)| \lesssim \left(\int_0^r U_0 ds\right) \exp\left(C \int_0^r V_0 ds\right) \lesssim \int_0^r U_0 ds \tag{3.188}$$

where $C > 0$ is a constant.

By (3.186) we can thus conclude that

$$|h_1(r)| + |k_1(r)| \lesssim \ln(r) \qquad \text{as} \quad r \longrightarrow +\infty \tag{3.189}$$

The above estimates imply that

$$2U_0V_0k_1, (3U_0^2 + V_0^2)h_1 \in L^1(\mathbb{R}^+)$$

and then integrating the second equation in (3.183) we get

$$h_1(r) \sim -\ln(r) \qquad \text{as} \quad r \longrightarrow +\infty \tag{3.190}$$

We now have to deal with remainder terms in (3.182).

In particular, we want to analyze the behavior of those terms on the time interval $\left(0, \frac{1}{\varepsilon}\right)$, thanks to a continuity argument based on the Gronwall inequality.

Let

$$\overline{r}_\varepsilon := \sup\left\{r \in \left[0, \varepsilon^{-1}\right) : |h_2(r,\varepsilon)| + |k_2(r,\varepsilon)| < \varepsilon^{-\frac{3}{2}}\right\} \tag{3.191}$$

Since $h_2(0,\varepsilon) = k_2(0,\varepsilon) = 0$, by continuity it is evident that

$$\overline{r}_\varepsilon > 0$$

As shown in the Appendix using the equations for h_2 and k_2 one gets the following estimates:

$$|h_2(r,\varepsilon)| + |k_2(r,\varepsilon)| \lesssim \frac{1}{\varepsilon}\ln\left(\frac{1}{\varepsilon}\right) + \int_0^r \left(V_0(s) + \varepsilon^2\right)\left(|h_2(s,\varepsilon)| + |k_2(s,\varepsilon)|\right) ds \tag{3.192}$$

for $0 < r < \overline{r}_\varepsilon \leqslant \frac{1}{\varepsilon}$.

The Gronwall estimates then imply that

$$|h_2(r,\varepsilon)| + |k_2(r,\varepsilon)| \lesssim \frac{1}{\varepsilon}\ln\left(\frac{1}{\varepsilon}\right) \exp\left(C \int_0^r \left(\varepsilon^2 + V_0(s)\right) ds\right) \tag{3.193}$$

for some $C > 0$. Since $r < \frac{1}{\varepsilon}$ and $V_0 \in L^1(\mathbb{R}^+)$ we thus obtain

$$|h_2(r,\varepsilon)| + |k_2(r,\varepsilon)| \lesssim \frac{1}{\varepsilon}\ln\left(\frac{1}{\varepsilon}\right) \tag{3.194}$$

Now, if we suppose that

$$\overline{r}_\varepsilon < \frac{1}{\varepsilon}$$

by (3.194) and by continuity there exists $\delta > 0$ such that

$$\frac{1}{\varepsilon}\ln\left(\frac{1}{\varepsilon}\right) \lesssim |h_2(r,\varepsilon)| + |k_2(r,\varepsilon)| \leqslant \varepsilon^{-\frac{3}{2}}$$

for all $r \in [\overline{r}_\varepsilon, \overline{r}_\varepsilon + \delta)$, thus contradicting the definition in (3.191).

Then there holds:

$$|h_2(r,\varepsilon)| + |k_2(r,\varepsilon)| < \varepsilon^{-\frac{3}{2}}, \qquad \forall r \in \left(0, \frac{1}{\varepsilon}\right) \tag{3.195}$$

Recall that the second equation in (3.182) reads as

$$V_\varepsilon(r) = V_0(r) + \varepsilon^2 k_1(r) + \varepsilon^4 k_2(r,\varepsilon)$$

By (3.194) and (3.175) we see that

$$V_0 = \mathcal{O}(\varepsilon^2) \quad , \quad k_2 = o(\varepsilon^2) \qquad \text{as} \quad r \to \left(\frac{1}{\varepsilon}\right)^-$$

Then by (3.190) we get

$$V_\varepsilon(r) \sim -\varepsilon^2 \ln\frac{1}{\varepsilon} \qquad \text{as} \quad r \to \left(\frac{1}{\varepsilon}\right)^- \tag{3.196}$$

Thus we have

$$V_\varepsilon(R_\varepsilon) = 0 \qquad \text{for some} \quad R_\varepsilon \in \left(0, \frac{1}{\varepsilon}\right) \tag{3.197}$$

In view of the scaling (3.170), we conclude that for large initial data $\lambda > 0$, the corresponding solution (u_λ, v_λ) of (3.149) has at least one node.

This proves the following (recall the definition (3.33))

Lemma 3.36. *The set A_0 is bounded.*

Then by (Lemma 3.33) we have that $I_0 \neq \emptyset$, that is the system (3.149) admits a solution without nodes, tending to (0,0) as $r \to +\infty$, which corresponds to a localised solution of equation (3.132). The exponential decay follows by (Lemma 3.31). This proves (Theorem 4.3).

Appendix

In this section we prove the estimates (3.192) for remainder terms in (3.182).

For the sake of brevity we only deal with k_2. The estimate for h_2 follows along the same lines with obvious modifications.

Inserting the ansatz (3.182) into the system (3.171), using equations (3.175) and (3.183) and imposing the initial condition we get the following equation

$$\begin{cases} \dfrac{d}{dr}k_2(r,\varepsilon) = K_0(r) + \varepsilon^2 K_2(r) + \varepsilon^4 K_4(r) + \varepsilon^6 K_6(r) + \varepsilon^8 K_8(r) \\ k_2(0,\varepsilon) = 0 \end{cases} \tag{3.198}$$

for all $\varepsilon > 0$. Note that the K^is do not depend on ε.

The terms in the r.h.s. are given by

$$\begin{cases} K_0 = -\left(2U_0^2 + V_0^2 + 2U_0V_0\right) h_2 - U_0\left(3h_1^2 + k_1^2\right) - 2V_0 h_1 k_1 - (m+\omega)h_1 \\ K_2 = -U_0\left(4h_1h_2 + 2k_1k_2\right) - (h_1^3 + h_1k_1^2) - 2V_0(h_1k_2 + k_1h_2) - (m+\omega)h_2 \\ K_4 = -\left(U_0(2h_2^2 + k_2^2) + 2V_0h_2k_2\right) - (2h_1k_1k_2 + 2h_1^2h_2 + k_1^2h_2) \\ K_6 = -h_1h_2^2 - k_1k_2^2 - h_1h_2^2 - k_1k_2h_2 \\ K_8 = -h_2^3 - h_2k_2^2 \end{cases} \tag{3.199}$$

Our aim is to estimate $|k_2(r,\varepsilon)|$ for $0 < r < \overline{r}$ (see (3.191)) and $0 < \varepsilon \ll 1$.

This is achieved integrating (3.198) and estimating the integral of the absolute value of each term in (3.199).

Remark that, by the definition of (U_0, V_0), (3.175)

$$2U_0^2 + V_0^2 + 2U_0V_0 \leqslant V_0 \in L^1(\mathbb{R}^+) \tag{3.200}$$

Moreover, (3.189) and (3.186) imply that $U_0\left(3h_1^2 + k_1^2\right) \notin L^1(\mathbb{R}^+)$ and then

$$\int_0^r U_0\left|3h_1^2 + k_1^2\right| ds \lesssim \int_1^{\frac{1}{\varepsilon}} \frac{\ln(s)}{s} ds \lesssim \varepsilon^{-\frac{1}{4}} \tag{3.201}$$

By the above remarks and (3.189), we have

$$V_0 h_1 k_1 \in L^1(\mathbb{R}^+) \tag{3.202}$$

and

$$\int_0^r |h_1| ds = \mathcal{O}(r \ln(r)), \qquad \text{as} \quad r \to +\infty \tag{3.203}$$

Collecting the above esimates we get

$$\int_0^r |K_0| ds \lesssim \int_0^r V_0 |h_2| ds + \varepsilon^{-1} |\ln(\varepsilon)| \tag{3.204}$$

The second term is estimated as follows.
Recall that

$$|h_2(r)| + |k_2(r)| \leqslant \varepsilon^{-\frac{3}{2}} \tag{3.205}$$

for $0 < r \leqslant \bar{r}$. Then by (3.200) we have

$$\int_0^r U_0 \, |4h_1 h_2 + 2k_1 k_2| \, ds \lesssim \varepsilon^{-\frac{3}{2}} \int_1^{\frac{1}{\varepsilon}} \frac{\ln(s)}{s} ds \lesssim \varepsilon^{-\frac{7}{4}} \tag{3.206}$$

Using again (3.189), it's not hard to see that

$$\int_0^r |h_1^3 + h_1 k_1^2| ds \lesssim \varepsilon^{-\frac{5}{4}} \tag{3.207}$$

Since

$$V_0 h_1, V_0 k_1 \in L^1(\mathbb{R}^+)$$

by (4.38) we have

$$\int_0^r V_0 \left(|h_1 k_2| + |k_1 h_2| \right) ds \lesssim \varepsilon^{-\frac{3}{2}} \tag{3.208}$$

We then conclude that

$$\int_0^r |K_2| ds \lesssim \varepsilon^{-\frac{7}{4}} + \int_0^r |h_2| ds \tag{3.209}$$

Let's turn to the third term.
By (3.200) and (4.38) and since $U_0(r) = \frac{2r}{4+r^2}$, we get

$$\int_0^r |U_0(2h_2^2 + k_2^2) + 2V_0 h_2 k_2| ds \lesssim \varepsilon^{-3} \int_1^{\frac{1}{\varepsilon}} U_0 ds \lesssim \varepsilon^{-3} |\ln(\varepsilon)| \tag{3.210}$$

Using (3.189) and (4.38) we can estimate

$$\int_0^{\overline{r}} |K_4| ds \lesssim \varepsilon^{-3} |\ln(\varepsilon)| + \varepsilon^{-\frac{5}{4}} \lesssim \varepsilon^{-3} |\ln(\varepsilon)| \tag{3.211}$$

All the terms appearing in K_6 have the same behavior, so that by (3.189),(4.38) and above estimates it's easy to see that

$$\int_0^r |K_6| ds \lesssim \varepsilon^{-4} |\ln(\varepsilon)| \tag{3.212}$$

Lastly, by (4.38) we can estimate

$$\int_0^r |K_8| ds \lesssim \varepsilon^{-\frac{11}{2}} \tag{3.213}$$

Combining (5.49,4.59,3.211,3.212,3.213), integrating (3.199) gives

$$|k_2(r,\varepsilon)| \lesssim \varepsilon^{-1} |\ln(\varepsilon)| + \int_0^r (V_0(s) + \varepsilon^2) |h_2(s,\varepsilon)| ds \tag{3.214}$$

Analogous estimates can be worked out for h_2, obtaining

$$|h_2(r,\varepsilon)| \lesssim \varepsilon^{-1} |\ln(\varepsilon)| + \int_0^r (V_0(s) + \varepsilon^2) |k_2(s,\varepsilon)| ds \tag{3.215}$$

and the claimed inequality (3.192) follows by summing up the last two estimates.

Chapter 4

A model for electron conduction in graphene

4.1 Introduction

This chapter is based on the paper [27].

Our aim is to study a quantum model for the transport of an electron gas in a graphene layer, in the case where particles are constrained in a bounded domain $\Omega \subset \mathbb{R}^2$.

As recalled in section 3.1, in [16] the authors gave a rigorous proof of the large, but finite, time-scale validity of a cubic Dirac equation, as a good approximation for the dynamics of the cubic nonlinear Schrödinger equation (NLS) with a honeycomb potential, in the weakly nonlinear regime. Their analysis indicates that an analogous result holds for the case of NLS with Hartree nonlinearity. We remark that ground state properties of graphene have been studied in [67] in the context of a Hartree-Fock model.

The (semi-classical) dynamics of electrons in a graphene layer can be described by the following NLS, the interaction being described by a self-consistent potential:

$$
\begin{cases} i\varepsilon\partial_t\Phi^\varepsilon = -\varepsilon^2\Delta\Phi^\varepsilon + V\left(\frac{x}{\varepsilon}\right)\Phi^\varepsilon + \varepsilon\kappa\left(\frac{1}{|x|} * |\Phi^\varepsilon|^2\right)\Phi^\varepsilon \\ \Phi^\varepsilon(0,x) = \Phi_0^\varepsilon(x) \end{cases} \tag{4.1}
$$

where V is a honeycomb potential and $\kappa \in \mathbb{R}$ is a coupling constant.

One expects that, as $\varepsilon \to 0$, the dynamics of WKB waves spectrally concentrated around a vertex of the Brillouin zone of the lattice (where the conical degeneracy occurs) can be effectively described by the following Dirac-Hartree equation:

$$\begin{cases} i\partial_t\varphi = -i\tilde{\sigma}\cdot\nabla\varphi + \kappa\left(\frac{1}{|x|} * |\varphi|^2\right)\varphi \\ \varphi(0,x) = \varphi_0(x) \end{cases} \tag{4.2}$$

where $\phi : \mathbb{R}_t \times \mathbb{R}^2_x \longrightarrow \mathbb{C}^2$, $\tilde{\sigma} := (\tilde{\sigma}_1, \tilde{\sigma}_2) = (\Lambda\sigma_1, \Lambda\sigma_2)$, with σ_i being the first two Pauli matrices

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{4.3}$$

and

$$\Lambda := \begin{pmatrix} \overline{\lambda} & 0 \\ 0 & \lambda \end{pmatrix}. \tag{4.4}$$

Here λ is a constant depending on the potential V (formula 4.1 in [56]).

In the above model, the particles can move in all the plane and the potential is the trace on the plane $\{z = 0\}$ of the 3-D Coulomb potential.

Remark 4.1. While the electrons in graphene are essentially confined in 2-D, the electric field clearly still acts in all three spatial dimensions. This justifies the choice of the 3-D Coulomb potential, given by the Riesz potential $(-\Delta)^{-\frac{1}{2}}$.

We consider the case where the electrons are constrained to a bounded domain $\Omega \subseteq \mathbb{R}^2$ modeling an electronic device. Following El-Hajj and Mehats [48], we define the self-consistent potential using the spectral resolution of $(-\Delta)^{\frac{1}{2}}$ with zero boundary conditions, in order to describe confinement of the electrons. In the same paper, the authors give a formal derivation of the potential $\mathcal{V}$ (recalled in the next section), starting from the 3-D Poisson equation. Moreover, in [48] El-Hajj and Mehats also prove local well-posedness for two models of electron transport in graphene. More precisely, they treat both the case where $\Omega = \mathbb{R}^2$ and $\Omega \subseteq \mathbb{R}^2$ is a bounded domain. In the latter case, they replace the Dirac operator by

$$\sigma_1(-\Delta)^{\frac{1}{2}} = \begin{pmatrix} 0 & (-\Delta)^{\frac{1}{2}} \\ (-\Delta)^{\frac{1}{2}} & 0 \end{pmatrix},$$

with zero Dirichlet data. It is easy to see that this operator displays a conical band dispersion structure and being off-diagonal it also couples valence and conduction bands, thus mimicking the Dirac operator. More details can be found in the references cited in [48].

Remark 4.2. In the case of graphene the zero-energy for the Dirac operator corresponds to the Fermi level. Then the positive part of the spectrum corresponds to massive conduction electrons, while the negative one to valence electrons.

Here we will instead work with the Dirac operator under suitable boundary conditions. It is well-known, in fact, that the Dirac operator, as well as general first order elliptic operators, is not self-adjoint with Dirichlet boundary conditions (see sections 8.2, 10.1 in [103] for a counterexample).

From now on $\Omega \subseteq \mathbb{R}^2$ will denote a smooth bounded open set.

Let $(e_n)_{n\in\mathbb{N}} \subseteq L^2(\Omega)$ be an orthonormal basis of eigenfunctions of the Dirichlet laplacian $(-\Delta)$, with associated eigenvalues $0 < \mu_n \uparrow +\infty$.

We define the potential $\mathcal{V}(\varphi)$ as

$$\mathcal{V}(\varphi) := \sum_{n\geqslant 0} \mu_n^{-\frac{1}{2}} \langle |\varphi|^2, e_n\rangle e_n \tag{4.5}$$

Thus $\mathcal{V}$ satisfies

$$(-\Delta)^{\frac{1}{2}}\mathcal{V} = |\varphi|^2 \qquad \text{in} \quad \Omega. \tag{4.6}$$

Working on a bounded domain, we need to choose *local* (for physical reasons) boundary conditions for the Dirac operator. We shall use *infinite mass boundary conditions* (see section 2.2), which have been employed in the Physics literature to model quantum dots in graphene (see [9] and reference therein).

Formally, infinite mass boundary conditions are defined imposing

$$P\psi := \frac{1}{2}(\mathbb{1}_2 - \tilde{\sigma}\cdot \boldsymbol{t})\psi = 0, \qquad \text{on} \quad \partial\Omega \tag{4.7}$$

where $\boldsymbol{t}$ is the tangent to the boundary and $\mathbb{1}_2$ is the unit matrix. It can be easily seen that such conditions make the Dirac operator

$$T := (-i\tilde{\sigma}\cdot\nabla)$$

symmetric on $L^2(\Omega, \mathbb{C}^2)$.

As explained in section 2.2 they actually belong to a larger class of local boundary conditions for the Dirac operator [9] employed in the theory of graphene, and which are related to M.I.T. and chiral boundary conditions (see [19] and references therein).

Proposition. *The unbounded operator $\mathcal{D}$ formally acting as $T := (-i\tilde{\sigma}\cdot\nabla)$ on $L^2(\Omega, \mathbb{C}^2)$*

is self-adjoint on the domain

$$D_\infty := \{\psi \in H^1(\Omega, \mathbb{C}^2) : (P \circ \gamma)\psi = 0\} \tag{4.8}$$

where P is the matrix defined in (4.7) and γ is the trace operator.

The model we are going to study thus is given by

$$\begin{cases} i\partial_t \phi = \mathcal{D}\phi + \kappa \mathcal{V}(\phi)\phi, & \text{in} \quad \mathbb{R}\times\Omega \\ \phi(0,x) = \phi_0(x) \end{cases} \tag{4.9}$$

Before stating our main theorem, we quickly review the spectral theory for the Dirac operator with infinite-mass boundary conditions, already recalled in section 2.2.

The compactness of the Sobolev embedding $H^1(\Omega, \mathbb{C}^2) \hookrightarrow L^2(\Omega, \mathbb{C}^2)$ gives that the spectrum of $\mathcal{D}$ is discrete. Moreover, the domain D_∞ is invariant with respect to the antiunitary transformation $\mathcal{U} := \sigma_1 \mathcal{C}$, where $\mathcal{C}$ is the complex conjugation on $L^2(\Omega, \mathbb{C}^2)$. Given $\varphi \in D_\infty$ we have

$$\mathcal{U}\mathcal{D}\varphi = -\mathcal{D}\mathcal{U}\varphi.$$

The above observations can be summarized in the following

Proposition. *The spectrum $\sigma(\mathcal{D}) \subseteq \mathbb{R}$ of $\mathcal{D}$ is purely discrete, symmetric and accumulates at $\pm\infty$.*

Let $(\psi_k)_{k\in\mathbb{Z}}$ be a Hilbert basis of $L^2(\Omega, \mathbb{C}^2)$ composed of eigenspinors of $\mathcal{D}$, and $(\lambda_k)_{k\in\mathbb{Z}}$ the associated eigenvalues, with $\lim_{k\to\pm\infty} \lambda_k = \pm\infty$.

It has been noted in the Physics literature that Dirac operators with infinite mass boundary condition are gapped. A rigorous proof has been recently given in [20], where the following result is proved.

Proposition. *For any $k \in \mathbb{Z}$ we have*

$$\lambda_k^2 \geqslant \frac{2\pi}{|\Omega|},$$

where $|\Omega|$ denotes the area of Ω.

We look for stationary solutions to the equation (4.9), that is, of the form

$$\phi(t,x) = e^{-i\omega t}\psi(x).$$

Plugging it into the equation one gets

$$(\mathcal{D} - \omega)\psi + \kappa\mathcal{V}(\psi)\psi = 0 \tag{4.10}$$

Our main result is the following:

Theorem 4.3. *(Multiple solutions for the Dirac-Hartree equation,[27]) Fix $\omega \notin \sigma(\mathcal{D})$. Then equation (4.10) admits infinitely many solutions in $C^\infty(\Omega, \mathbb{C}^2)$ satisfying the boundary condition (4.7).*

We remark that a variational proof of existence and multiplicity for 3D Maxwell-Dirac and Dirac-Coulomb equations can be found in [51]. Those results have been improved in [1]. The case of subritical Dirac equations on compact spin manifolds has been treated in [71], for nonlinearity with polynomial growth, and using a Galerkin-type approximation. Our proof is variational and based on direct arguments. The present work has been inspired by the above mentioned articles and by the papers [16, 48].

For the sake of simplicity we will restrict ourselves to $\omega \in (-\lambda_1, \lambda_1)$.

Remark 4.4. Without loss of generality, we can choose $\kappa < 0$. In particular, we take $\kappa = -1$. The case $\kappa > 0$ follows considering the functional

$$\mathcal{L}(\psi) := -\mathcal{I}(\psi)$$

(see below).

Solutions to (4.10) will be obtained as critical points of the functional

$$\mathcal{I}(\psi) = \frac{1}{2}\int_\Omega \langle(\mathcal{D} - \omega)\psi, \psi\rangle - \frac{1}{4}\int_\Omega \mathcal{V}(\psi)|\psi|^2 \tag{4.11}$$

which is defined and of class C^2 on the Hilbert space

$$X := \left\{\psi \in L^2(\Omega, \mathbb{C}^2) : \|\psi\|^2_X := \sum_{k\in\mathbb{Z}} |\lambda_k - \omega||\langle\psi, \psi_k\rangle|^2 < \infty\right\} \tag{4.12}$$

endowed with the scalar product

$$\langle\phi, \psi\rangle_X := \langle\phi, \psi\rangle_{L^2} + \sum_{k\in\mathbb{Z}} |\lambda_k - \omega|\langle\phi, \psi_k\rangle_{L^2}\overline{\langle\psi, \psi_k\rangle}_{L^2}.$$

In the proof of Theorem 1 in [19] it is shown that for some $C > 0$ there holds

$$\|\varphi\|_{H^1} \leqslant C(\|\varphi\|_{L^2} + \|T\varphi\|_{L^2}) \tag{4.13}$$

for all $\varphi \in D_\infty$, that is, for spinors in the operator domain.

This implies that the H^1-norm and the quantity in brackets in the r.h.s. of (4.13) are equivalent on D_∞. Then interpolating between $L^2(\Omega, \mathbb{C}^2)$ and D_∞, one gets the following

Remark 4.5. The X-norm above defined and the $H^{\frac{1}{2}}$-norm are equivalent on the space X. This will be repeatedly used in the sequel in connection with Sobolev embeddings.

We can thus split X as the direct sum of the positive and the negative spectral subspaces of $(\mathcal{D} - \omega)$:

$$X = X^+ \oplus X^- \tag{4.14}$$

Accordingly we will write $\psi = \psi^+ + \psi^-$.

The functional (5.22) then takes the form

$$\mathcal{I}(\psi) = \frac{1}{2}\left(\|\psi^+\|_X^2 - \|\psi^-\|_X^2\right) - \frac{1}{4}\int_\Omega \mathcal{V}(\psi)|\psi|^2 \tag{4.15}$$

Smoothness of the solutions will follow by standard bootstrap arguments.

Remark 4.6. Despite the term in (5.22) involving the potential being 4-homogeneous we can take advantage of regularization property of $(-\Delta)^{-\frac{1}{2}}$, thus avoiding compactness issues related to the limiting Sobolev embedding $X \hookrightarrow L^4$. This is in contrast with the equations studied in the previous chapter, where we considered Kerr-like cubic nonlinearities. We dealt with the lack of compactness through a suitable radial ansatz, reducing the proof to dynamical systems arguments.

In the sequel, we will denote X-norm and the L^p-norm of a spinor ψ by $\|\psi\|$ and $\|\psi\|_p$, respectively. Occasionally, we will also omit the domain of definition of functions, denoting L^p and Sobolev spaces.

4.1.1 A formal derivation of $\mathcal{V}$.

Our argument follows the one given in [48]. It is included here for the reader's convenience.

We show how the potential $\mathcal{V}$ is obtained as the trace on the plane $\{z = 0\}$ of the solution of the 3D Poisson equation. We consider only the simple case where the boundary is connected to a cilindrical perfect conductor.

In our model, the electrons are constrained to a bounded domain

$$\Omega \times \{0\} \subseteq \mathbb{R}^3.$$

Then the 3D potential satisfies

$$(-\partial_z^2 - \Delta)V^{3D} = \underbrace{n(x)\delta(z)}_{density}, \qquad (x, z) \in \Omega \times \mathbb{R} \tag{4.16}$$

where $\Delta = \partial_x^2 + \partial_y^2$ and $\delta(z)$ is the Dirac mass.

We also impose the boundary conditions

$$V^{3D}(x, z) = 0, \quad (x, z) \in \partial\Omega \times \mathbb{R}, \qquad V^{3D} \xrightarrow{z\to\pm\infty} 0.$$

Let $(e_k)_{k\in\mathbb{N}} \subseteq L^2(\Omega)$ be an orthonormal basis of eigenfunctions of the Dirichlet laplacian $(-\Delta)$, with associated eigenvalues $0 < \mu_k \uparrow +\infty$.

Projecting equation onto e_n, for each $n \in \mathbb{N}$, gives

$$-\partial_z^2 V_k^{3D} + \mu_n V_k^{3D} = n_k \delta(z)$$

with $V_k^{3D}(z) = \int_\Omega V^{3D}(x, z)e_k(x)dx$ and $n_k = \int_\Omega n(x)e_k(x)dx$.

Solving the last equation one gets

$$V^{3D}(x, z) = \frac{1}{2}\sum_{k\mathbb{N}} n_k e_k(x) \frac{e^{-\sqrt{\mu_k}|z|}}{\sqrt{\mu_k}} \qquad (x, z) \in \Omega \times \mathbb{R}$$

and thus

$$\mathcal{V}(x) = V^{3D}(x,0) = \frac{1}{2}\sum_{k\mathbb{N}} (\mu_k)^{-\frac{1}{2}} n_k e_k(x) = \frac{1}{2}(-\Delta)^{-\frac{1}{2}} n.$$

4.2 Existence of multiple solutions

4.2.1 The variational argument

This section is devoted to the proof of our main theorem. The strategy consists in exploiting the $\mathbb{Z}_2$-symmetry of the functional using topological arguments, in order to get multiple solutions. Our argument proceeds suitably splitting the Hilbert space X according to the spectral decomposition of the operator $(\mathcal{D} - \omega)$. This allows us to define an increasing sequences of critical values $c_j \uparrow +\infty$ for the action functional (5.22). Compactness of critical sequences is proved exploiting the regularizing effect of $(-\Delta)^{-\frac{1}{2}}$.

It is easy to see that the functional $\mathcal{I}$ is even :

$$\mathcal{I}(-\psi) = \mathcal{I}(\psi), \quad \forall\psi \in X$$

and this allows us to prove a multiplicity result using a straightforward generalization of the fountain theorem, well-known for semi-definite functionals (see, e.g. [125]). It in turn relies on the following infinite-dimensional Borsuk-Ulam theorem [105].

Let H be a Hilbert space.

Definition 4.7. We say that $\Phi : H \longrightarrow H$ is a *Leray-Schauder map* (LS-map) if it is of the form

$$\Phi = I + K \tag{4.17}$$

where I is the identity and K is a compact operator.

Theorem 4.8. *(Borsuk-Ulam in Hilbert spaces) Let $Y \leqslant H$ be a codimension one subspace of H and $\mathcal{U}$ be a symmetric (i.e. $\mathcal{U} = -\mathcal{U}$) bounded neighborhood of the origin. If $\Phi : \partial\mathcal{U} \longrightarrow Y$ is an odd LS-map, then there exists $x \in \partial\mathcal{U}$ such that $\Phi(x) = 0$.*

The proof of the above theorem is achieved approximating the compact map by finite rank operators and using the finite-dimensional Borsuk-Ulam theorem, as shown in [105].

Consider an Hilbert basis $(e_k)_{k\in\mathbb{Z}}$ of H. For $j \in \mathbb{Z}$ we define

$$H_1(j) := \overline{span\{e_k\}}_{-\infty}^{k=j}, \quad H_2(j) := \overline{span\{e_k\}}_{k=j}^{+\infty} \tag{4.18}$$

Given $0 < r_j < \rho_j$ we set

$$B(j) := \{\psi \in \mathbf{H}_1(j) \ : \ \|\psi\| \leqslant \rho_j\}$$

$$S(j) := \{\psi \in \mathbf{H}_1(j) \ : \ \|\psi\| = \rho_j\}$$

$$N(j) := \{\psi \in \mathbf{H}_2(j) \ : \ \|\psi\| = r_j\}$$

Let $\mathcal{L} \in C^1(H, \mathbb{R})$ be an even functional of the form

$$\mathcal{L}(\psi) = \frac{1}{2}\langle L\psi, \psi\rangle + F(\psi) \tag{4.19}$$

where

$$L : H_1(j) \oplus H_2(j) \longrightarrow H_1(j) \oplus H_2(j)$$

is linear, bounded and self-adjoint and dF is a compact map.

It is a well-known result (see,e.g. ([102], Appendix) and [114]) that such a functional admits an odd pseudo-gradient flow of the form

$$\eta(t,*) = \Lambda(t,*) + K(t,*) = \Lambda_{1,j}(t,*) \oplus \Lambda_{2,j}(t,*) + K(t,*), \tag{4.20}$$

where $\Lambda_{i,j}(t,*) : \mathbf{H}_i(j) \to \mathbf{H}_i(j)$ is an isomorphism ($i = 1,2$), and $K(t,*)$ is a compact map.

Theorem 4.9. *(Fountain theorem) With the above notations, define the min-max level*

$$c_j := \inf_{\gamma\in\Gamma(j)} \sup \mathcal{L}(\gamma(1, B(j))) \tag{4.21}$$

where $\Gamma(j)$ is the class of maps $\gamma \in C^0([0,1] \times B(j), H)$ such that

$$\gamma(t,\psi) = \psi, \qquad \forall (t,\psi) \in [0,1] \times S(j)$$

and which are homotopic to the identity through a family of odd maps of the form (4.20). If there holds

$$\inf_{\psi\in N(j)} \mathcal{L}(\psi) =: b_j > a_j := \sup_{\psi\in S(j)} \mathcal{L}(\psi), \tag{4.22}$$

then $c_j \geqslant b_j$ and there exists a Cerami sequence $(\psi^j_n)_{n\in\mathbb{N}} \subseteq H$, that is

$$\begin{cases} \mathcal{L}(\psi^j_n) \longrightarrow c_j \\ (1 + \|\psi^j_n\|)d\mathcal{L}(\psi^j_n) \xrightarrow{H^*} 0 \qquad as \quad n \longrightarrow \infty \end{cases} \tag{4.23}$$

where H^* is the dual space of H.

Moreover, if Cerami sequences are pre-compact, then c_j is a critical value.

Proof. The proof follows by a standard deformation argument (see [102, 114]). However, we quickly sketch the proof for the convenience of the reader. More details can be found in the above-mentioned references.

Fix $j \in \mathbb{N}$. We first show that

$$c_j \geqslant b_j > a_j, \tag{4.24}$$

where c_j is the min-max value defined in (5.43) and b_j is as in (4.22). To this aim, we need to prove the intersection property

$$\gamma(1, B(j)) \cap N(j) \neq \emptyset$$

for any $\gamma \in \Gamma(j)$. Since γ is odd in the second variable, $\gamma(1{,}0) = 0$ and the set

$$\mathcal{U} = \{u \in B(j) : \|\gamma(1,u)\| < r\} \tag{4.25}$$

is a bounded neighborhood of the origin such that $-\mathcal{U} = \mathcal{U}$.

Let $P : H \longrightarrow Y := \overline{span\{e_k\}_{-\infty}^{k=j-1}}$ be the projection. Consider the map $(P \circ \gamma)(1,*) : \partial\mathcal{U} \longrightarrow Y$. We have to prove that the equation

$$(P \circ \gamma)(1,u) = 0 \tag{4.26}$$

admits a solution $u_0 \in \partial\mathcal{U}$.

Recall that $\gamma(1,*)$ is of the form (4.20). Then (4.26) is equivalent to

$$u + \underbrace{(P \circ \Lambda^{-1}(1,*) \circ K)}_{\text{compact}}(1,u) = 0$$

and the claim follows by the Borsuk-Ulam theorem (Theorem 4.8).

We claim that there is a *Palais-Smale sequence* at level c_j (PS_{c_j} sequence, for short), that is, there exists a sequence $(\psi_n^j)_{n\in\mathbb{N}} \subseteq H$ such that there holds

$$\begin{cases} \mathcal{L}(\psi_n^j) \longrightarrow c_j \\ d\mathcal{L}(\psi_n^j) \xrightarrow{H^*} 0 \qquad \text{as} \quad n \longrightarrow \infty. \end{cases} \tag{4.27}$$

If this is not the case, since $\mathcal{L}$ is of class C^2 this implies that there exist $\delta, \varepsilon > 0$ such that

$$\|d\mathcal{L}(\psi)\| \geqslant \delta > 0 \tag{4.28}$$

for $\psi \in \{c_j - \varepsilon \leqslant \mathcal{L} \leqslant c_j + \varepsilon\}$.

By (5.43) it follows that there exists $\gamma_\varepsilon \in \Gamma(j)$ such that

$$\sup \mathcal{L}(\gamma_\varepsilon(1, B(j))) \leqslant c_j + \varepsilon.$$

Following the construction explained, for instance, in [102, 114], one can construct a suitable vector field (a *pseudo-gradient vector field* for $\mathcal{L}$) whose flow is as in (4.20) and such that $\frac{d}{dt}\mathcal{L}(\eta(t,\psi)) \leqslant 0$, $\forall (t,\psi) \in [0{,}1] \times H$. Moreover, combining (4.24,4.28) and choosing $\varepsilon > 0$ small, one can also obtain $\eta(t,\psi) = \psi$, for $\psi \notin \{c_j - \varepsilon \leqslant \mathcal{L} \leqslant c_j + \varepsilon\}$, and that $\eta(1,\cdot)$ maps $\{\mathcal{L} \leqslant c_j + \varepsilon\}$ to $\{\mathcal{L} \leqslant c_j - \varepsilon\}$. Combining those observations one gets that $\eta \circ \gamma_\epsilon \in \Gamma(j)$. But then

$$\sup \mathcal{L}(\eta \circ \gamma_\epsilon(1, B(j))) \leqslant c_j - \varepsilon, \tag{4.29}$$

contradicting the definition of the min-max value (5.43). This proves the existence of a PS_{c_j}-sequence $(\psi^j_n)_n$. Moreover, applying Ekeland's variational principle [47] this can be promoted to a Cerami sequence, thus concluding the proof. □

Our aim is to apply the fountain theorem to the functional $\mathcal{I}$. First of all, we need to study the geometry of the functional $\mathcal{I}$.

Proposition. *The functional*

$$\mathcal{I}(\psi) = \frac{1}{2}\int_\Omega \langle(\mathcal{D} - \omega)\psi, \psi\rangle - \frac{1}{4}\int_\Omega \mathcal{V}(\psi)|\psi|^2$$

is of the form (4.19).

Proof. The term involving the potential is 4-homogeneous, but we can avoid compactness issues related to the critical Sobolev embedding $H^{\frac{1}{2}}(\Omega, \mathbb{C}^2) \hookrightarrow L^4(\Omega, \mathbb{C}^2)$ thanks to the regularizing properties of $(-\Delta)^{-\frac{1}{2}}$, as shown in Proposition (4.2.2). □

For each $j \geqslant 1$, consider the splitting

$$X = X_1(j) \oplus X_2(j) = \left(\overline{span\{\psi_k\}}^{j}_{k=-\infty}\right) \oplus \left(\overline{span\{\psi_k\}}^{+\infty}_{k=j}\right) \tag{4.30}$$

where $(\psi_k)_{k\in\mathbb{Z}}$ is an orthonormal basis of eigenspinors of $\mathcal{D}$.

Lemma 4.10. *Let $j \geqslant 1$, there exists $\rho_j > 0$ such that $\mathcal{I}(\psi) \leqslant 0$, for $\psi \in X_1(j)$ and $\|\psi\| \geqslant \rho_j$.*

Proof. Let $\psi \in X_1(j)$ be such that $\|\psi\| \geqslant \rho_j > 0$. Recall that

$$\psi = \psi^- + \psi^+ \in Y := X^- \oplus span\{e_k\}^{k=1}_{j}.$$

Suppose that

$$\|\psi^-\| \geqslant \|\psi^+\|. \tag{4.31}$$

It is immediate from (4.15) that $\mathcal{I}(\psi) \leqslant 0$.

Now assume

$$\|\psi^+\| \geqslant \|\psi^-\|. \tag{4.32}$$

We claim that there exists $C = C(j) > 0$ such that

$$\mathcal{Q}(\psi) := \int_\Omega \mathcal{V}(\psi)|\psi|^2 \geqslant C\|\psi\|^4 \tag{4.33}$$

for all $\psi \in Y$ satisfying (4.32).

Suppose the claim is false. Then arguing by contradiction and by the 4-homogeneity of $\mathcal{Q}$, there exists a sequence $(\psi_n)_{n\in\mathbb{N}} \subseteq Y$ satisfying (4.32), and such that $\|\psi_n\| = 1$ and

$$\mathcal{Q}(\psi_n) \longrightarrow 0, \qquad \text{as} \quad n \to +\infty.$$

Notice that (4.32) implies that

$$\|\psi_n^+\| \geqslant \frac{1}{\sqrt{2}} \tag{4.34}$$

Up to subsequences, we can assume that there exists $\psi_\infty \in Y$ such that ψ_n^- weakly converges to ψ_∞^-, while ψ_n^+ strongly converges to ψ_∞^+, the latter sequence lying in a finite-dimensional space. Thus there holds

$$\|\psi_\infty^+\| \geqslant \frac{1}{\sqrt{2}}. \tag{4.35}$$

Since $\mathcal{Q}$ is continuous and convex it also is weakly lower semi-continuous, and then

$$\mathcal{Q}(\psi_\infty) = 0.$$

This implies that

$$\psi_\infty = \psi_\infty^+ + \psi_\infty^- = 0$$

and thus

$$\psi_\infty^+ = 0 \tag{4.36}$$

ψ_∞^- and ψ_∞^+ being orthogonal, contradicting (4.35).

Then , given (4.33), we have

$$\mathcal{I}(\psi) \leqslant \|\psi^+\| - \|\psi^-\| - C\|\psi\|^4 \tag{4.37}$$

for all $\psi \in Y$ such that (4.32) holds. Thus $\mathcal{I}(\psi) \leqslant 0$, for $\rho_j > 0$ large enough.

□

Lemma 4.11. *For* $1 \leqslant p < 4$ *define*

$$\beta_{j,p} := \sup\{\|\psi\|_p : \psi \in X_2(j), \|\psi\| = 1\}.$$

Then $\beta_{j,p} \longrightarrow 0$ *as* $j \to \infty$.

Proof. By definition, for each $j \geqslant 1$ there exists $\psi_j \in X_2(j)$ such that $\|\psi_j\| = 1$ and $\frac{1}{2}\beta_{j,p} < \|\psi_j\|_p$. The compactness of the Sobolev embedding implies that, up to subsequences, $\psi_j \rightharpoonup \psi$ weakly in X and $\psi_j \longrightarrow \psi$ strongly in $L^p(\Omega, \mathbb{C}^2)$. It is evident that $\psi = 0$. Then

$$\frac{1}{2}\beta_{j,p} < \|\psi_j\|_p \longrightarrow 0.$$

□

The above result allows us to prove the following:

Lemma 4.12. *There exists* $r_j > 0$ *such that*

$$b_j := \inf\{\mathcal{I}(\psi) : \psi \in X_2(j), \|\psi\| = r_j\} \longrightarrow +\infty$$

as $j \longrightarrow +\infty$.

Proof. By the Hölder inequality, we get

$$\int_\Omega \mathcal{V}(\psi)|\psi|^2 \leqslant \left(\int_\Omega |\psi|^3\right)^{\frac{2}{3}} \left(\int_\Omega \mathcal{V}(\psi)^3\right)^{\frac{1}{3}} \leqslant C\|\psi\|_3^4. \tag{4.38}$$

Recall that $\mathcal{V}(\psi) := (-\Delta)^{-\frac{1}{2}}(|\psi|^2)$. Since $|\psi|^2 \in L^{\frac{3}{2}}(\Omega, C^2)$, and $(-\Delta)^{-\frac{1}{2}}$ sends $L^{\frac{3}{2}}(\Omega, \mathbb{C}^2)$ into $W^{1,\frac{3}{2}}(\Omega, \mathbb{C}^2) \hookrightarrow L^3(\Omega, \mathbb{C}^2)$, we easily get (4.38).

Take $\psi \in X_2(j)$ such that $\|\psi\| = r$. Then by (4.38) and Lemma 4.11 we have

$$\begin{aligned} \mathcal{I}(\psi) &= \frac{1}{2}\int_\Omega \langle(\mathcal{D} - \omega)\psi, \psi\rangle - \int_\Omega \mathcal{V}(\psi)|\psi|^2 \\ &\geqslant \frac{1}{2}\|\psi\|^2 - \frac{1}{2}\|\psi\|_2^2 - C\|\psi\|_3^4 \\ &\geqslant \frac{1}{2}r^2 - \frac{1}{2}r^2\beta_{j,2}^2 - Cr^4\beta_{j,3}^4 \\ &\geqslant \frac{1}{4}r^2 - C\beta_{j,3}^4 r^4 \end{aligned} \tag{4.39}$$

where we used the fact that $\beta_{j,2}^2 \leqslant \frac{1}{2}$.

The function $r \mapsto \frac{1}{4}r^2 - C\beta_{j,3}^4 r^4$ attains its maximum at $r = (8C\beta_{j,3}^4)^{-\frac{1}{2}}$. Then taking $r_j := (8C\beta_{j,3}^4)^{-\frac{1}{2}}$ we get

$$b(j) \geqslant (64C\beta_{j,3}^3)^{-1} \longrightarrow +\infty$$

and this concludes the proof. ☐

The above results allow us to apply the Fountain theorem (Theorem 4.9) to the functional $\mathcal{I}$. We thus get the existence of a sequence of min-max values

$$c_j \longrightarrow +\infty, \qquad \text{as} \quad j \to +\infty, \tag{4.40}$$

and, for each $j \in \mathbb{N}$, of a Cerami sequence $(\psi_j^n)_{n\in\mathbb{N}} \in X$:

$$\begin{cases} \mathcal{I}(\psi_j^n) \longrightarrow c_j \\ (1 + \|\psi_j^n\|)d\mathcal{I}(\psi_j^n) \xrightarrow{X^*} 0 \qquad \text{as} \quad n \longrightarrow \infty \end{cases} \tag{4.41}$$

Lemma 4.13. *Cerami sequences for $\mathcal{I}$ are pre-compact .*

Proof. Let $(\psi_n) \subseteq X$ be an arbitrary Cerami sequence for $\mathcal{I}$.

Then

$$\begin{cases} \mathcal{I}(\psi_n) \longrightarrow c \\ (1 + \|\psi_n\|)(\mathcal{D}\psi_n - \mathcal{V}(\psi_n)\psi_n) \xrightarrow{X^*} 0 \qquad \text{as} \quad n \longrightarrow \infty \end{cases} \tag{4.42}$$

for some $c > 0$.

The second condition in (4.42) implies that

$$\int_\Omega \langle \mathcal{D}\psi_n, \psi_n \rangle - \int_\Omega \mathcal{V}(\psi_n)|\psi_n|^2 \longrightarrow 0. \tag{4.43}$$

Combining (4.43) and the first line in (4.42) one gets

$$\|\mathcal{V}(\psi_n)\|^2_{\mathring{H}^{\frac{1}{2}}} = \int_\Omega |(-\Delta)^{\frac{1}{4}}\mathcal{V}(\psi_n)|^2 = \int_\Omega \mathcal{V}(\psi_n)|\psi_n|^2 \longrightarrow 2c. \tag{4.44}$$

By the Sobolev embedding $(\mathcal{V}(\psi_n))_{n\in\mathbb{N}}$ is thus bounded in L^4. Moreover, since $(-\Delta)^{-\frac{1}{2}}$ is positivity-preserving (see section 4.2.2), (4.44) implies that $(\mathcal{V}(\psi_n)|\psi_n|^2)_{n\in\mathbb{N}}$ is bounded in L^1.

By the above remarks, writing

$$\mathcal{V}(\psi_n)|\psi_n| = \underbrace{\Big(\mathcal{V}(\psi_n)|\psi_n|^2\Big)^{\frac{1}{2}}}_{L^2-bounded}\underbrace{(\mathcal{V}(\psi_n))^{\frac{1}{2}}}_{L^8-bounded} \tag{4.45}$$

and by the Hölder inequality, we easily get that $(\mathcal{V}(\psi_n)\psi_n)_{n\in\mathbb{N}}$ is bounded in $L^{\frac{8}{5}}$. The second line of (4.42) gives

$$\psi_n = \psi_n^1 + \psi_n^2 := (\mathcal{D}-\omega)^{-1}(\mathcal{V}(\psi_n)\psi_n) + o(1), \qquad \text{in} \quad H^{\frac{1}{2}}(\Omega,\mathbb{C}^2) \tag{4.46}$$

It is immediate to see that $(\psi_n^1)_{n\in\mathbb{N}}$ is bounded in $W^{1,\frac{8}{5}} \hookrightarrow H^{\frac{1}{2}}$, and thus $(\psi_n)_{n\in\mathbb{N}}$ is bounded in $H^{\frac{1}{2}}$.

Up to subsequences, there exists $\psi_\infty \in X$ such that $\psi_n \rightharpoonup \psi_\infty$ weakly in X and $\psi_n \to \psi_\infty$ strongly in L^p for all $1 \leqslant p < 4$.

Since $(\psi_n)_{n\in\mathbb{N}}$ is a Cerami sequence, there holds

$$o(1) = \langle d\mathcal{I}(\psi_n), \psi_n^+ - \psi_\infty^+\rangle = \int_\Omega \langle \mathcal{D}\psi_n^+, \psi_n^+ - \psi_\infty^+\rangle - \int_\Omega \mathcal{V}(\psi_n)\langle \psi_n, \psi_n^+ - \psi_\infty^+\rangle. \tag{4.47}$$

Moreover, the Hölder inequality gives

$$\begin{aligned}
\left|\int_\Omega \mathcal{V}(\psi_n)\langle\psi_n, \psi_n^+ - \psi_\infty^+\rangle\right| &\leqslant \int_\Omega \mathcal{V}(\psi_n)|\psi_n||\psi_n^+ - \psi_\infty^+| \\
&\leqslant \|\mathcal{V}(\psi_n)|\psi_n|\|_2 \|\psi_n^+ - \psi_\infty^+\|_2 \\
&\leqslant \|\mathcal{V}(\psi_n)\|_6 \|\psi_n\|_3 \|\psi_n^+ - \psi_\infty^+\|_2 \\
&\leqslant C\|\psi_n^+ - \psi_\infty^+\|_2
\end{aligned} \tag{4.48}$$

where in the last line we used the fact that (ψ_n) is bounded in $H^{\frac{1}{2}} \hookrightarrow L^3$ and that $(\mathcal{V}(\psi_n))_{n\in\mathbb{N}}$ is L^6-bounded. Combining (4.47) and (4.48) we get

$$\int_\Omega \langle \mathcal{D}\psi_n^+, \psi_n^+ - \psi_\infty^+\rangle = o(1) \tag{4.49}$$

On the other hand, for any $\eta^+ \in X^+$, there holds

$$\int_\Omega \langle \mathcal{D}\eta^+, \eta^+\rangle \geqslant (1 + (\lambda_1)^{-1})\|\eta^+\|^2 \tag{4.50}$$

as it can be easily checked. By (4.50) and (4.49) we thus obtain

$$\|\psi_n^+ - \psi_\infty^+\|^2 \leqslant C\int_\Omega \langle \mathcal{D}(\psi_n^+ - \psi_\infty^+), \psi_n^+ - \psi_\infty^+\rangle = o(1). \tag{4.51}$$

An analogous argument gives

$$\|\psi_n^- - \psi_\infty^-\|^2 = o(1) \tag{4.52}$$

thus proving the pre-compactness of Cerami sequences. □

Our main theorem (Theorem 4.3) is thus proved, as the regularity of solutions follows by standard bootstrap techniques, exploiting the regularization property of $(-\Delta)^{-\frac{1}{2}}$.

4.2.2 Auxiliary results

This section contains some auxiliary results used in the proof of our main theorem.
Compactness of dF.

Lemma 4.14. *Let $(Y, \|\cdot\|_Y)$ be a uniformly convex Banach space and consider a sequence $(y_n)_{n\in\mathbb{N}} \subseteq Y$. Suppose that $y_n \rightharpoonup y$ weakly in Y and $\|y_n\|_Y \to \|y\|_Y$.*

Then $y_n \longrightarrow y$ strongly in Y, as $n \to +\infty$.

See [32] for a proof. The above lemma allows us to prove the following

Proposition. *Let $(\psi_n)_{n\in\mathbb{N}} \subseteq X$ be a sequence such that $\psi_n \to \psi \in X$ strongly in L^p, for all $1 \leqslant p < 4$.*

Then, up to a subsequence $|\psi_n|^2 \to |\psi|^2$ strongly in $L^{\frac{3}{2}}$, as $n \to +\infty$.

Proof. We have

$$\||\psi_n|^2\|_{\frac{3}{2}} = \|\psi_n\|_3^2 \longrightarrow \|\psi\|_3^2 = \||\psi|^2\|_{\frac{3}{2}} \tag{4.53}$$

as $n \to +\infty$, since $\psi_n \to \psi$ strongly in L^3.

Moreover, it is easy to see that

$$\||\psi_n|^2\|_{\frac{3}{2}} = \|\psi_n\|_3^2 \leqslant C \tag{4.54}$$

and thus, up to a subsequence, $|\psi_n|^2 \rightharpoonup |\psi|^2$ weakly in $L^{\frac{3}{2}}$.

Then the claim follows by Lemma 4.14, L^p spaces being uniformly convex for $1 < p < +\infty$ (see,e.g. [32]). . □

Consider the map $F : X \longrightarrow \mathbb{R}$, defined as

$$F(\psi) := \frac{1}{4}\int_\Omega \mathcal{V}(\psi)|\psi|^2 \tag{4.55}$$

It can be easily seen that the differential $dF : X \longrightarrow X^*$ acts as follows:

$$\langle dF(\psi), \varphi\rangle_{X^*\times X} = \int_\Omega \mathcal{V}(\psi)\Re(\psi\overline{\varphi}), \qquad \forall \psi, \varphi \in X, \tag{4.56}$$

where $\Re(\cdot)$ denotes the real part of a complex number.

Proposition. *The differential dF is compact.*

Proof. Let $(\psi_n)_{n\in\mathbb{N}} \subseteq X$ be a bounded sequence. Then the compactness of the Sobolev embedding $H^{\frac{1}{2}}(\Omega, \mathbb{C}^2) \hookrightarrow L^p(\Omega, \mathbb{C}^2)$, for $1 \leqslant p < 4$, implies that, up to subsequences, $\psi_n \to \psi \in X$, strongly in L^p.

Take $\varphi \in X$ with $\|\varphi\| \leqslant 1$. We then have

$$\begin{aligned} \left|\int_\Omega \left(\mathcal{V}(\psi_n)\psi_n - \mathcal{V}(\psi)\psi\right)\overline{\varphi}\right| &\leqslant \int_\Omega |(\mathcal{V}(\psi_n)\psi_n - \mathcal{V}(\psi_n)\psi)\overline{\varphi}| \\ &\quad + \int_\Omega |(\mathcal{V}(\psi_n)\psi - \mathcal{V}(\psi)\psi)\overline{\varphi}| \end{aligned} \tag{4.57}$$

We estimate the first term in the r.h.s. as follows.

Applying the Cauchy-Schwarz inequality we get

$$\begin{aligned} \int_\Omega |(\mathcal{V}(\psi_n)\psi_n - \mathcal{V}(\psi_n)\psi)\overline{\varphi}| &\leqslant \left(\int_\Omega |\mathcal{V}(\psi_n)\varphi|^2\right)^{\frac{1}{2}} \left(\int_\Omega |\psi_n - \psi|^2\right)^{\frac{1}{2}} \\ &\leqslant \|\varphi\|_4 \|\mathcal{V}(\psi_n)\|_4 \|\psi_n - \psi\|_2 \\ &\leqslant C\|\psi_n - \psi\|_2 \longrightarrow 0 \end{aligned} \tag{4.58}$$

for $n \to +\infty$, using the fact that $(-\Delta)^{-\frac{1}{2}}$ maps continuously L^2 to $H^1 \hookrightarrow L^4$, and $\mathcal{V}(\psi) = (-\Delta)^{-\frac{1}{2}}|\psi|^2$.

For the second term in (4.57), we use again the Cauchy-Schwarz inequality and get

$$\begin{aligned} \int_\Omega |(\mathcal{V}(\psi_n)\psi - \mathcal{V}(\psi)\psi)\varphi| &\leqslant \left(\int_\Omega |\psi\varphi|^2\right)^{\frac{1}{2}} \left(\int_\Omega |\mathcal{V}(\psi_n) - \mathcal{V}(\psi)|^2\right)^{\frac{1}{2}} \\ &\leqslant \|\varphi\|_4 \|\psi\|_4 \|\mathcal{V}(\psi_n) - \mathcal{V}(\psi)\|_2 \\ &\leqslant C\|\mathcal{V}(\psi_n) - \mathcal{V}(\psi)\|_2 \longrightarrow 0 \end{aligned} \tag{4.59}$$

as $n \to +\infty$, since $\mathcal{V}(\psi_n) = (-\Delta)^{-\frac{1}{2}}|\psi_n|^2 \in W^{1,\frac{3}{2}}(\Omega, \mathbb{C}^2) \hookrightarrow L^2(\Omega, \mathbb{C}^2)$ and $|\psi_n|^2 \to |\psi|^2$ strongly in $L^{\frac{3}{2}}$, as shown in Prop.(5.48).

Thus combining (4.58) and (4.59) we have

$$\left|\int_\Omega \left(\mathcal{V}(\psi_n)\psi_n - \mathcal{V}(\psi)\psi\right)\overline{\varphi}\right| \longrightarrow 0 \tag{4.60}$$

uniformly with respect to φ, as $n \to +\infty$. $\square$

$(-\Delta)^{-\frac{1}{2}}$ is positivity-preserving. For the sake of brevity we will only sketch the argument, referring to the mentioned references for more details.

Recall that $-\Delta$ is the Dirichlet laplacian on $L^2(\Omega)$, with domain $H_0^1(\Omega)$.

The starting point is the following identity of L^2-operators:

$$(-\Delta)^{-\frac{1}{2}} = \frac{1}{\sqrt{\pi}} \int_0^{+\infty} e^{-t^2\Delta} dt. \tag{4.61}$$

Indeed, let $(e_n)_{n\in\mathbb{N}} \subseteq L^2(\Omega)$ be a Hilbert basis of eigenfunctions of $-\Delta$, with associated eigenvalues $0 < \mu_n \uparrow +\infty$.

For any $n \in \mathbb{N}$ the operator on the r.h.s. of (4.61) acts on each e_n as the multiplication operator by the function

$$\frac{1}{\sqrt{\pi}} \int_0^{+\infty} e^{-t^2\mu_n} dt = \frac{1}{\sqrt{\mu_n}}. \tag{4.62}$$

To prove the claim it is thus sufficient to prove that the heat kernel $e^{-s\Delta}$ is positivity-preserving. This follows from the

Theorem 4.15. *(First Beurling-Deny criterion) Let $L \geqslant 0$ be a self-adjoint operator on $L^2(\Omega)$. Extend $\langle u, Lu\rangle_{L^2}$ to all L^2 by setting it equal to $+\infty$, when u does not belong to the form-domain of L. The following are equivalent:*

- *e^{-sL} is positivity-preserving for all $s > 0$;*
- *$\langle |u|, L|u|\rangle_{L^2} \leqslant \langle u, Lu\rangle_{L^2}, \quad \forall u \in L^2(\Omega)$.*

A proof of the above result can be found in ([104], Theorem XIII.50).

Taking $L = -\Delta$, the second condition in the above theorem corresponds to the well-known fact that for any $u \in H_0^1(\Omega)$ there holds

$$|\nabla |u|| \leqslant |\nabla u| \qquad \text{a.e. in} \quad \Omega$$

and then

$$\langle |u|, L|u|\rangle_{L^2} = \int_\Omega |\nabla |u||^2 \leqslant \int_\Omega |\nabla u|^2 = \langle u, Lu\rangle_{L^2}$$

(see Theorem 6.1 in [83]). This concludes the proof.

Chapter 5

Nonlinear Dirac equations on quantum graphs with localized nonlinearities

The present chapter is based on the forthcoming paper [29]. This is a joint work with Raffaele Carlone and Lorenzo Tentarelli. We study the nonlinear Dirac (NLD) equation on noncompact metric graphs with localized Kerr nonlinearities, in the case of Kirchhoff-type conditions at the vertices. Precisely, we discuss existence and multiplicity of the bound states (arising as critical points of the NLD action functional) and we prove that, in the L^2-subcritical case, they converge to bound states of the NLS equation in the nonrelativistic limit, for a wide range of parameters.

5.1 Introduction

The investigation of evolution equations on metric graphs (see, e.g., Figure 5.1) has become very popular nowadays as they are assumed to represent effective models for the study of the dynamics of physical systems confined in branched spatial domains. A specific attention has been addressed to the *focusing* nonlinear Schrödinger (NLS) equation, i.e.

$$\imath\partial_t v = -\Delta v - |v|^{p-2}\, v, \qquad p \geqslant 2, \tag{5.1}$$

with suitable vertex conditions, as it is supposed to well approximate (for $p = 4$) the behavior of Bose-Einstein condensates in ramified traps (see, e.g., [65] and references therein).

From the mathematical point of view, the discussion has been mainly focused on the

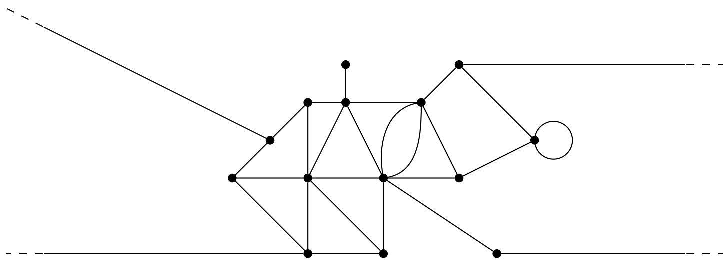

Figure 5.1. a general noncompact metric graph.

study of the stationary solutions of (5.1), namely functions of the form $v(t,x) = e^{-i\lambda t}\,u(x)$, with $\lambda \in \mathbb{R}$, that solve the stationary version of (5.1), i.e.

$$-\Delta u - |u|^{p-2}\,u = \lambda u\,,$$

with vertex conditions of δ-type. In particular, the most investigated subcase has been that of the *Kirchhoff* vertex conditions, which impose at each vertex:

(i) continuity of the function (for details see (5.16)),

(ii) "balance" of the derivatives (for details see (5.17)).

For a short bibliography limited to the case of noncompact metric graphs with a finite number of edges (which is the one discussed here) we refer the reader to, e.g., [3, 4, 5, 6, 35, 36, 82, 96, 97] and the references therein.

Following [64, 95], a particular attention has also been devoted to a simplified version of the model where the nonlinearity localized on the *compact core* $\mathcal{K}$ of the graph, which is the subgraph consisting of all the bounded edges (see, for instance, Figure 5.2); namely,

$$-\,\Delta u - \chi_{\mathcal{K}}|u|^{p-2}\,u = \lambda u \tag{5.2}$$

with Kirchhoff vertex conditions. Here $\chi_{\mathcal{K}}$ denotes the characteristic function of $\mathcal{K}$. This problem has been studied in the L^2-subcritical case in [111, 112, 117], while some new results on the L^2-critical case have been presented in [46].

Remark 5.1. We also mention some interesting results on the problem of the bound states on compact graphs. For a purely variational approach we recall, e.g., [45], whereas for a bifurcation approach we refer to, e.g., [88].

As a further development, in the last years also the study of the Dirac operator on metric graphs has generated a growing interest (see, e.g., [8, 24, 33, 101]). In particular,

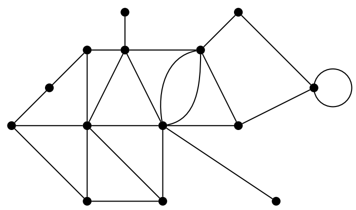

Figure 5.2. the compact core of the graph in Figure 5.1.

[106] proposed (although in the toy case of the *infinite 3-star* graph, depicted in Figure 5.3) the study of the *nonlinear* Dirac equation on networks, namely (5.1) with the laplacian replaced by the Dirac operator

$$\mathcal{D} := -\imath c \frac{d}{dx} \otimes \sigma_1 + mc^2 \otimes \sigma_3, \tag{5.3}$$

where $m > 0$ and $c > 0$ are two parameters representing the *mass* of the generic particle of the system and the *speed of light* (respectively), and σ_1 and σ_3 are the *Pauli matrices*, i.e.

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{and} \qquad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{5.4}$$

and with the wave function v replaced by the spinor $\chi := (\chi^1, \chi^2)^T$. Precisely, [106] suggests the investigation of stationary solutions, that is $\chi(t,x) = e^{-i\omega t}\,\psi(x)$, with $\omega \in \mathbb{R}$, that solve

$$\mathcal{D}\psi - |\psi|^{p-2}\,\psi = \omega\psi\,. \tag{5.5}$$

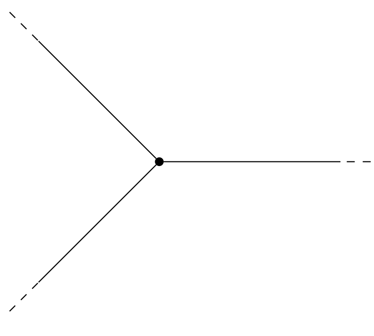

Figure 5.3. infinite 3-star graph.

In this chapter, we discuss the case of (5.5) with localized nonlinearity (or, equivalently, the Dirac analogue of (5.2)), namely

$$\mathcal{D}\psi - \chi_{\mathcal{K}}|\psi|^{p-2}\,\psi = \omega\psi\,.$$

The reduction to this simplified model, as in the Schrödinger case, is due to the fact that one assumes that nonlinearity affects only the compact core, while since localized stationary solutions decay exponentially on half-lines the nonlinear terms become negligible outside a compact part of the graph. However, the investigation of the case with the "extended" nonlinearity, i.e. (5.5), will be discussed in a forthcoming paper.

In the sequel we will tacitly make use of the properties of the operator $\mathcal{D}$ with Kirchoff-type conditions, summarized in Section 2.3. For the convenience of the reader, we recall here the main result of that section.

Proposition 5.2. *The Dirac operator* $\mathcal{D}$ (5.3) *with Kirchoff-type vertex conditions* (2.49),(2.50) *is self-adjoint on* $L^2(\mathcal{G},\mathbb{C}^2)$ *with domain given by* (2.48)*. Its spectrum is given by*

$$\sigma(\mathcal{D}) = (-\infty, -mc^2] \cup [mc^2, +\infty).$$

5.2 Definition of the form domain

The standard cases of the Dirac operator $\mathbb{R}^d, d = 1{,}2{,}3$ do not require any further remark on the associated quadratic form, which can be easily defined using the Fourier transform (see e.g. [54]). Unfortunately, in the framework of (noncompact) metric graphs this tool is not available and hence it is necessary to resort to the *Spectral Theorem*. This represents a more abstract way to diagonalize the Dirac operator and consequently define the associated quadratic form $\mathcal{Q}_{\mathcal{D}}$ using *real interpolation theory* [14, 7]. Define the space

$$Y := \Big[L^2(\mathcal{G},\mathbb{C}^2), \mathrm{dom}(\mathcal{D})\Big]_{\frac{1}{2}}\,, \tag{5.6}$$

namely the interpolated space of order 1/2 between L^2 and the domain of the Dirac operator. First, we note that Y is a closed subspace of

$$H^{1/2}(\mathcal{G},\mathbb{C}^2) := \bigoplus_{e\in\mathrm{E}} H^{1/2}(I_e)\otimes\mathbb{C}^2,$$

with respect to the norm induced by $H^{1/2}(\mathcal{G},\mathbb{C}^2)$. Indeed, $\mathrm{dom}(\mathcal{D})$ is clearly a closed subspace of $H^1(\mathcal{G},\mathbb{C}^2)$ and there results (arguing edge by edge) that

$$H^{1/2}(\mathcal{G},\mathbb{C}^2) = \Big[L^2(\mathcal{G},\mathbb{C}^2), H^1(\mathcal{G},\mathbb{C}^2)\Big]_{\frac{1}{2}},$$

so that the closedness of Y follows by the very definition of interpolation spaces . As a consequence, by Sobolev embeddings there results that

$$Y \hookrightarrow L^p(\mathcal{G},\mathbb{C}^2), \qquad \forall p \geqslant 2, \tag{5.7}$$

and that, in addition, the embegging in $L^p(\mathcal{K},\mathbb{C}^2)$ is compact, due to the compactness of $\mathcal{K}$. On the other hand, there holds

$$\mathrm{dom}(\mathcal{Q}_{\mathcal{D}}) = Y, \tag{5.8}$$

and hence the form domain inherits all the properties pointed out before, which are in fact crucial in the sequel.

Let us quickly sketch the proof of (5.8). As already remarked, it can be achieved combining the Spectral Theorem and real interpolation theory.

One of the most commonly used forms of the Spectral Theorem states, roughly speaking, that every self-adjoint operator on a Hilbert space is isometric to a multiplication operator on a suitable L^2-space. In this sense the operator can be "diagonalized" in an abstract way.

Theorem 5.3. *([103, thm. VIII.4]) Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$ with domain $\mathrm{Dom}(H)$. There exists a measure space (M,μ), with μ a finite measure, a unitary operator*

$$U : \mathcal{H} \longrightarrow L^2(M, d\mu), \tag{5.9}$$

and a real valued function f on M, a.e. finite, so that

1. *$\psi \in \mathrm{Dom}(H)$ if and only if $f(\cdot)(U\psi)(\cdot) \in L^2(M,d\mu)$,*
2. *if $\varphi \in U[\mathrm{Dom}\, H]$, then $(UHU^{-1})(m) = f(m)\varphi(m), \quad \forall m \in M$.*

The above theorem essentially says that H is isometric to the multiplication operator by f (still denoted by the same symbol) on the space $L^2(M,d\mu)$, whose domain is given by

$$\mathrm{Dom}(f) := \Big\{\varphi \in L^2(M,d\mu) : f(\cdot)\varphi(\cdot) \in L^2(M,d\mu)\Big\}. \tag{5.10}$$

endowed with the norm

$$\|\varphi\|_1^2 := \int_M (1 + f(m)^2)\varphi(m)^2 d\mu(m) \tag{5.11}$$

The form domain of f has an obvious explicit definition, as f is a multiplication operator. Anyway, it can be recovered using real interpolation theory as follows. We follow the presentation given in [7, 14], to which the reader can refer for more details.

Consider the Hilbert spaces $\mathcal{H}_0 := L^2(M, d\mu)$ with the norm $\|x\|_0 := \|x\|_{L^2(d\mu)}$, and $\mathcal{H}_1 := \mathrm{Dom}(f)$. Then $\mathcal{H}_1 \subset \mathcal{H}_0$. Let us define the following quadratic version of Peetre's *K-functional*

$$K(t, x) := \inf\left\{\|x_0\|_0^2 + t\|x_1\|_1^2 : x = x_0 + x_1, x_0 \in \mathcal{H}_0, x_1 \in \mathcal{H}_1\right\}. \tag{5.12}$$

The squared norm $\|x\|_1^2$ is a densely defined quadratic form on $\mathcal{H}_0$, represented by

$$\|x\|_1^2 = \langle (1 + f^2(\cdot))x, x\rangle_0, \tag{5.13}$$

where $\langle \cdot, \cdot\rangle_0$ is the scalar product of $\mathcal{H}_0$.

By standard arguments (see e.g. [14] or [7, Ch. 7] and references therein) the intermediate spaces $\mathcal{H}_1 \subset [\mathcal{H}_0, \mathcal{H}_1]_\theta \subset \mathcal{H}_0$, $0 < \theta < 1$, are given by the elements $x \in \mathcal{H}_0$ such that the following quantity is finite:

$$\int_0^\infty \left(t^{-\theta}K(t, x)\right)\frac{dt}{t} < \infty. \tag{5.14}$$

Then for the spaces $\mathcal{H}_\theta := [\mathcal{H}_0, \mathcal{H}_1]_\theta$ there holds

$$\|x\|_\theta^2 = \langle (1 + f^2(\cdot))^\theta x, x\rangle_0.$$

Then for $\theta = \frac{1}{2}$ one recovers the form domain of the operator f. Now taking $H = \mathcal{D}$ and $\mathcal{H} = L^2(\mathcal{G}, \mathbb{C}^2)$ with domain as in (2.48), we conclude that the space defined in (5.6) is exactly the form domain of $\mathcal{D}$, and there holds $Y = U^{-1}\mathcal{H}_{\frac{1}{2}}$.

Finally, for the sake of simplicity (and following the literature on the NLD equation), we denote throughout the form domain by Y, in view of (5.8), and

$$\mathcal{Q}_\mathcal{D}(\psi) = \frac{1}{2}\int_\mathcal{G} \langle \psi, \mathcal{D}\psi\rangle\, dx, \qquad \text{and} \qquad \mathcal{Q}_\mathcal{D}(\psi, \varphi) = \frac{1}{2}\int_\mathcal{G} \langle \psi, \mathcal{D}\varphi\rangle\, dx,$$

with $\langle \cdot\, , \cdot \rangle$ denoting the euclidean sesquilinear product of $\mathbb{C}^2$, since this does not give rise to misunderstandings. In particular, as soon as ψ and/or φ are smooth enough (e.g., if they belong to the operator domain) the previous expressions gain an actual meaning as Lebesgue integrals.

We also recall that in the sequel we denote duality pairings by $\langle \cdot | \cdot \rangle$ (the function spaces involved being clear from the context).

Remark 5.4. Note that the the combination between spectral theorem and interpolation theory is (to the best of our knowledge) the sole possibility to define the quadratic form, since also classical duality arguments fail due to the fact that it is not true in general that $H^{-1/2}(\mathcal{G}, \mathbb{C}^2)$ is the topological dual of $H^{1/2}(\mathcal{G}, \mathbb{C}^2)$ (due to the presence of bounded edges).

5.2.1 Main results

We can now, state the main results of this chapter. Preliminarily, we give the definition of bound state of the NLD and of the NLS equations on noncompact metric graphs with localized nonlinearities.

Definition (Bound states of the NLDE)**.** Let $\mathcal{G}$ be a noncompact metric graph with nonempty compact core $\mathcal{K}$ and let $p \geqslant 2$. Then, a *bound state of the NLDE* with Kirchhoff-type vertex conditions and nonlinearity localized on $\mathcal{K}$ is a spinor $0 \not\equiv \psi \in \mathrm{dom}(\mathcal{D})$ for which there exists $\omega \in \mathbb{R}$ such that

$$\mathcal{D}_e\psi_e - \chi_{\mathcal{K}}|\psi_e|^{p-2}\psi_e = \omega\psi_e, \qquad \forall e \in \mathrm{E}, \tag{5.15}$$

with $\chi_{\mathcal{K}}$ the characteristic function of the compact core $\mathcal{K}$.

Definition (Bound states of the NLSE)**.** Let $\mathcal{G}$ be a noncompact metric graph with nonempty compact core $\mathcal{K}$, and let $p \geqslant 2$ and $\alpha > 0$. Then, a *bound state of the NLSE* equation with Kirchhoff vertex conditions and focusing nonlinearity localized on $\mathcal{K}$ is a function $0 \not\equiv u \in H^2(\mathcal{G})$ that satisfies

$$u_e(\mathrm{v}) = u_f(\mathrm{v}), \qquad \forall e, f \succ \mathrm{v}, \qquad \forall \mathrm{v} \in \mathcal{K}, \tag{5.16}$$

$$\sum_{e \succ v} \frac{du_e}{dx_e}(\mathrm{v}) = 0, \qquad \forall \mathrm{v} \in \mathcal{K}, \tag{5.17}$$

where $\frac{du_e}{dx_e}(\mathrm{v})$ stands for $u_e'(0)$ or $-u_e'(\ell_e)$ according to whether x_e is equal to 0 or ℓ_e at v, and for which there exists $\lambda \in \mathbb{R}$ such that

$$-u_e'' - \alpha\chi_{\mathcal{K}}|u_e|^{p-2}u_e = \lambda u_e, \qquad \forall e \in \mathrm{E}. \tag{5.18}$$

Remark 5.5. We recall that conditions (5.16)&(5.17) make the laplacian self-adjoint on $\mathcal{G}$ and are called Kirchhoff conditions. We also recall that the parameters ω and λ are usually referred to as *frequencies* of the bound states of the NLDE and NLSE (respectively), whereas α is usually connected to the scattering length of the particles.

Theorem 5.6 (Existence and multiplicity of the bound states [29]). *Let $\mathcal{G}$ be a noncompact metric graph with nonempty compact core and let $m, c > 0$ and $p \geqslant 2$. Then, for every $\omega \in (-mc^2, mc^2)$ there exists infinitely (distinct) pairs of bound states of frequency ω of the NLDE.*

Some comments are in order. First of all, to the best of our knowledge this is the first rigorous result on the stationary solutions of the nonlinear Dirac equation on metric graphs.

On the other hand, some relevant differences can be observed with respect to the Schrödinger case. Bound states of Theorem 5.6 arise (as we will extensively show in the next section) as critical points of the functional

$$\mathcal{L}(\psi) := \frac{1}{2}\int_{\mathcal{G}} \langle \psi, (\mathcal{D} - \omega)\psi \rangle \, dx - \frac{1}{p}\int_{\mathcal{K}} |\psi|^p \, dx.$$

However, due to the spectral properties of $\mathcal{D}$, the kinetic part of $\mathcal{L}$ (that is, the quadratic form associated with $\mathcal{D}$) is unbounded from below even if one constrains the functional to the set of the spinors with fixed L^2-norm, in contrast to the NLS functional. As a consequence, no minimization can be performed and, hence, the extensions of the direct methods of calculus of variations developed for the Schrödinger case are useless.

Furthermore, such a kinetic part is also strongly indefinite, so that the functional possesses a significantly more complex geometry with respect to the NLS case, thus calling for more technical tools of critical point theory.

Finally, the spinorial structure of the problem as well as the implicit definition of the kinetic part of the functional, whose domain is not embedded in $L^\infty(\mathcal{G}, \mathbb{C}^2)$, prevent the (direct) use of some useful tools developed for the NLS on graphs such as, for instance, rearrangements and "graph surgery".

In view of these issues, in the proof of Theorem 5.6 we rather adapted some techniques from the literature on the NLDE on standard noncompact domains. Anyway, the fact that we are dealing with a nonlinearity defined only on a compact part of the graph makes the study of the geometry of the functional a bit more delicate (see Lemma 5.11). For the same reason, the uniform H^1-boundedness needed to study the non relativistic limit of bound states is achieved in different steps (see Sec.5.4).

The second (and main) result of this section, on the other hand, shows the connection between the NLDE and the NLSE, suggested by the physical interpretation of the two models.

Before presenting the statement, we recall that, by the definition of $\mathcal{D}$, the bound states obtained via Theorem 5.6 depend in fact on the speed of light c. As a consequence, they should be meant as bound states of frequency ω of the NLDE *at speed of light* c.

Theorem 5.7 (Nonrelativistic limit of the bound states [29])**.** *Let $\mathcal{G}$ be a noncompact metric graph with nonempty compact core, and let $m > 0$, $p \in (2,6)$ and $\lambda < 0$. Consider real sequences $(c_n), (\omega_n)$ such that*

$$0 < c_n, \omega_n \to +\infty, \tag{5.19}$$

$$\omega_n < mc_n^2, \tag{5.20}$$

$$\omega_n - mc_n^2 \longrightarrow \frac{\lambda}{m}, \tag{5.21}$$

as $n \to +\infty$. If $\{\psi_n = (\psi_n^1, \psi_n^2)^T\}$ is a bound state of frequency ω_n of the NLDE (5.15) *at speed of light c_n, then up to subsequences there holds*

$$\psi_n^1 \longrightarrow u \qquad \textit{and} \qquad \psi_n^2 \longrightarrow 0 \qquad \textit{in} \quad H^1(\mathcal{G}),$$

as $n \to +\infty$, where u is a bound state of frequency λ of the NLSE (5.18) *with $\alpha = 2m$.*

First, we recall that the expression "speed of light c_n, with $c_n \to \infty$" has to be meant as if it is bigger and bigger with respect to the proper scale of the phenomenon one is focusing on. In addition, for any choices for which the proof of Theorem 5.7 holds, there results that the parameter α in the NLSE solved by the limit function u is equal to $2m$.

The main interest of Theorem 5.7 arises from the fact that it suggests that the two models provided by the NLDE and the NLSE are indistinguishable at those scales where the relativistc effects become negligible. Hence our result provides a mathematical evidence to these intuitive guesses.

Moreover, we point out that Theorem 5.7, in contrast to Theorem 5.6, holds only for a fixed range of power exponents, namely the so-called L^2-subcritical case $p \in (2,6)$. However, this is the only range of powers for which multiplicity results are known for the NLSE (see [111]). On the other hand, these results are parametrized by the L^2 norm of the wave function while Theorem 5.7 is parametrized by the frequency and hence (in some sense) it presents as a byproduct a new result for the NLSE.

Remark 5.8. We also mention that Theorem 5.6 and Theorem 5.7 can be proved, without significant modifications, also in the case of more general nonlinearities, by means of several ad hoc assumptions. We limit ourselves to the power case in this presentation for the aim of simplicity.

5.3 Existence of infinitely many bound states

In this Section we prove Theorem 5.6. Note that, since the parameter c here does not play any role, we set $c = 1$ throughout the section. In addition, in the sequel (unless stated otherwise) we always tacitly assume that the mass parameter m is positive, the frequency $\omega \in (-m, m)$, the power of the nonlinearity $p > 2$ and that $\mathcal{G}$ is a noncompact metric graph with nonempty compact core.

5.3.1 Preliminary results

The first point is to prove that the bound states coincide with the critical points of the C^2 action functional $\mathcal{L} : Y \to \mathbb{R}$ defined by

$$\mathcal{L}(\psi) = \frac{1}{2}\int_{\mathcal{G}} \langle \psi, (\mathcal{D} - \omega)\psi \rangle \, dx - \frac{1}{p}\int_{\mathcal{K}} |\psi|^p \, dx. \tag{5.22}$$

Recall that the spectrum of $\mathcal{D}$ is given by

$$\sigma(\mathcal{D}) = (-\infty, -m] \cup [m, +\infty). \tag{5.23}$$

Proposition. *A spinor is a bound state of frequency ω of the NLDE if and only if it is a critical point of $\mathcal{L}$.*

Proof. One can easily see that a bound state of frequency ω of the NLDE is a critical point of $\mathcal{L}$. Let us prove, therefore, the converse.

Assume that ψ is a critical point of $\mathcal{L}$, namely that $\psi \in Y$ and

$$\langle d\mathcal{L}(\psi)|\varphi \rangle = \int_{\mathcal{G}} \langle \psi, (\mathcal{D} - \omega)\phi \rangle \, dx - \int_{\mathcal{K}} |\psi|^{p-2} \langle \psi, \varphi \rangle \, dx = 0, \qquad \forall \phi \in Y. \tag{5.24}$$

Now, for any fixed edge $e \in \mathrm{E}$, if one chooses

$$\phi = \begin{pmatrix} \phi^1 \\ 0 \end{pmatrix}, \qquad \text{with} \quad 0 \neq \phi^1 \in C_0^\infty(I_e) \tag{5.25}$$

(namely, ϕ^1 possesses the sole component ϕ^1_e, which is a test function of I_e), then

$$\imath \int_{I_e} \psi_e^2\,(\overline{\phi}_e^1)'\,dx_e = \int_{I_e} \underbrace{\left[(m-\omega)\psi_e^1 + \chi_{-\mathcal{K}}|\psi_e|^{p-2}\psi_e^1\right]}_{\in L^2(I_e)} \overline{\phi}_e^1\,dx_e,$$

so that $\psi_e^2 \in H^1(I_e)$ and an integration by parts yields the first line of (5.15). On the other hand, simply exchanging the role of ϕ^1 and ϕ^2 in (5.25), one can see that $\psi_e^1 \in H^1(I_e)$ and satisfies the second line of (5.15), as well.

It is then left to prove that ψ fulfills (2.49) and (2.50). First, fix a vertex v of the compact core and choose

$$\mathrm{dom}(\mathcal{D}) \ni \phi = \begin{pmatrix} \phi^1 \\ 0 \end{pmatrix}, \qquad \text{with} \qquad \phi^1(\mathrm{v}) = 1, \qquad \phi(\mathrm{v}') = 0 \quad \forall \mathrm{v}' \in \mathcal{K},\ \mathrm{v}' \neq \mathrm{v}.$$

Integrating by parts in (5.24) and using (5.15), there results

$$\sum_{e \succ \mathrm{v}} \phi_e^1(\mathrm{v})\psi_e^2(\mathrm{v})_\pm = 0$$

and, hence, ψ^2 satisfies (2.50) (recall the meaning of $\psi_e^2(\mathrm{v})_\pm$ explained in Definition 2.3.2). On the other hand, let v be a vertex of the compact core with degree greater than or equal to 2 (for vertices of degree 1 (2.49) is satisfied for free). Morevoer, let

$$\mathrm{dom}(\mathcal{D}) \ni \phi = \begin{pmatrix} 0 \\ \phi^2 \end{pmatrix}, \qquad \text{with} \qquad \phi_{e_1}^2(\mathrm{v})_\pm = -\phi_{e_2}^2(\mathrm{v})_\pm, \qquad \phi_e^2(\mathrm{v}) = 0 \quad \forall e \neq e_1, e_2,$$

where e_1 and e_2 are two edges incident at v, and $\phi_e^2 \equiv 0$ on each edge not incident at v. Again, integrating by parts in (5.24) and using (5.15),

$$\phi_{e_1}^2(\mathrm{v})_\pm \psi_{e_1}^1(\mathrm{v}) + \phi_{e_2}^2(\mathrm{v})_\pm \psi_{e_2}^1(\mathrm{v}) = 0.$$

Then, repeating the procedure for any pair of edges incident at v one gets (2.49).

Finally, iterating the same arguments on all the vertices one concludes the proof. □

Remark 5.9. In addition to Proposition 5.3.1, it is worth mentioning that, due to the linear behavior outside the compact core, the bound states are known explicitly on the half-lines. Pecisely, if $e \in \mathrm{E}$ is a half-line with starting point v, then

$$
\begin{cases} \psi_e^1(x_e) = -\imath\, \psi_e^1(\mathrm{v})\sqrt{\dfrac{m+\omega}{m-\omega}}\, e^{-\sqrt{m^2-\omega^2}x_e} \\ \psi_e^2(x_e) = \psi_e^2(\mathrm{v})e^{-\sqrt{m^2-\omega^2}x_e} \end{cases}, \qquad x_e \in [0,\infty). \tag{5.26}
$$

The second preliminar step is to prove that the functional $\mathcal{L}$ possesses a so-called *linking geometry* ([54, 114]), since this is the main tool in order to prove the existence of Palais-Smale sequences.

Recall that, according to (5.23) we can decompose the form domain Y as the orthogonal sum of the positive and negative spectral subspaces for the operator $\mathcal{D}$, i.e.

$$
Y = Y^+ \oplus Y^-.
$$

As a consequence, every $\psi \in Y$ can be written as $\psi = P^+\psi + P^-\psi =: \psi^+ + \psi^-$, where $P^\pm$ are the orthogonal projectors onto $Y^\pm$. In addition one can find an equivalent (but more convenient) norm for Y, i.e.

$$
\|\psi\| := \|\sqrt{|\mathcal{D}|}\psi\|_{L^2}, \qquad \forall \psi \in Y.
$$

Remark 5.10. Borel functional calculus for self-ajoint operators [103, Thm. VIII.5] allows to define the operators $|\mathcal{D}|^\alpha$, $\alpha > 0$, and more general operators of the form $f(\mathcal{D})$, where f is a Borel function on $\mathbb{R}$.

In view of the previous remarks and using again the Spectral theorem, the action functional (5.22) can be rewritten as follows

$$
\mathcal{L}(\psi) = \frac{1}{2}(\|\psi^+\|^2 - \|\psi^-\|^2) - \frac{\omega}{2}\int_{\mathcal{G}} |\psi|^2 - \frac{1}{p}\int_{\mathcal{K}} |\psi|^p\, dx, \tag{5.27}
$$

which is the best form in order to prove that $\mathcal{L}$ has in fact a linking geometry (see e.g. [114, Sec. II.8]).

Lemma 5.11. *For every $N \in \mathbb{N}$ there exist $R = R(N,p) > 0$ and an N-dimensional space $Z_N \subset Y^+$ such that*

$$
\mathcal{L}(\psi) \leqslant 0, \qquad \forall \psi \in \partial\mathcal{M}_N, \tag{5.28}
$$

where

$$
\partial\mathcal{M}_N = \Big\{\psi \in \mathcal{M}_N : \|\psi^-\| = R \quad \text{or} \quad \|\psi^+\| = R\Big\}.
$$

and

$$\mathcal{M}_N := \Big\{\psi \in Y : \|\psi^-\| \leqslant R \quad \text{and} \quad \psi^+ \in Z_N \quad \text{with} \quad \|\psi^+\| \leqslant R\Big\}. \tag{5.29}$$

Proof. Let e be a bounded edge, associated with the segment $I_e = [0, \ell_e]$, and let V be the space of the spinors

$$\eta = \begin{pmatrix} \eta^1 \\ 0 \end{pmatrix}, \qquad \text{with} \quad \eta^1 \in C_0^\infty(I_e),$$

which is clearly a subset of $\mathrm{dom}(\mathcal{D})$ and hence of Y. Moreover, a simple computation shows that

$$\int_{\mathcal{G}} \langle \eta, \mathcal{D}\eta\rangle \, dx = m \int_{\mathcal{G}} |\eta_1|^2 \, dx \tag{5.30}$$

and thus, in view of (5.27), if $\eta_1 \neq 0$ then $\eta^+ \neq 0$.

Assume first that $\dim V^+ = \infty$, where $V^+ = V \cap Y^+$. For every fixed $N \in \mathbb{N}$, choose N linearly independent spinors $\eta_1^+, ..., \eta_N^+ \in V^+$ and set $Z_N := \mathrm{span}\{\eta_1^+, ..., \eta_N^+\}$. As a consequence, if $\psi \in \partial\mathcal{M}_N$, then $\psi = \varphi + \xi$ with $\varphi \in Y^-$ and $\xi \in Z_N$, so that

$$\mathcal{L}(\psi) = \mathcal{L}(\varphi + \xi) = \frac{1}{2}\left(\|\xi\|^2 - \|\varphi\|^2\right) - \frac{1}{p}\int_{\mathcal{K}} |\varphi + \xi|^p \, dx.$$

It is clear that, if $\|\varphi\| \geqslant \|\xi\|$, then

$$\mathcal{L}(\varphi + \xi) \leqslant -\int_{\mathcal{K}} |\varphi + \xi|^p \, dx \leqslant 0$$

If, on the contrary, $\|\xi\| \geqslant \|\varphi\|$, then some further effort is required. Since $\psi \in \partial\mathcal{M}_N$, $\|\xi\| = R$ and thus

$$\mathcal{L}(\varphi + \xi) \leqslant \frac{R^2}{2} - \frac{1}{p}\int_{\mathcal{K}} |\varphi + \xi|^p \, dx.$$

From the Hölder inequality

$$\int_{\mathcal{K}} |\varphi + \xi|^2 \leqslant \ell^{\frac{p-2}{p}} \left(\int_{\mathcal{K}} |\varphi + \xi|^p \, dx\right)^{\frac{2}{p}} \tag{5.31}$$

(recall that $\ell = |\mathcal{K}|$) and hence

$$\mathcal{L}(\varphi + \xi) \leqslant \frac{R^2}{2} - \frac{\ell^{\frac{p(2-p)}{4}}}{p} \left(\int_{\mathcal{K}} |\varphi + \xi|^2 \, dx\right)^{\frac{p}{2}}. \tag{5.32}$$

Now, by definition, $\xi = \sum_{j=1}^N \lambda_j \eta_j^+$, for some $\lambda_j \in \mathbb{C}$. On the other hand, denoting by η_j^-

the spinors such that $\eta_j^- + \eta_j^+ =: \eta_j \in V$, since $\varphi \in Y^-$, there results that $\varphi = \varphi^\perp + \chi$, with $\chi := \sum_{j=1}^N \lambda_j \eta_j^-$ and $\varphi^\perp$ the orthogonal complement of χ in Y^-. Therefore, as $\varphi^\perp$ is orthogonal to χ and ξ in $L^2(\mathcal{G}, \mathbb{C}^2)$,

$$\int_{\mathcal{G}} |\varphi + \xi|^2\, dx = \int_{\mathcal{G}} |\varphi^\perp|^2\, dx + \int_{\mathcal{G}} |\xi + \chi|^2\, dx; \tag{5.33}$$

while, as $\xi + \chi = \sum_{j=1}^N \lambda_j \eta_j$ vanishes outside $I \subset \mathcal{K}$,

$$\int_{\mathcal{G}} |\varphi + \xi|^2\, dx = \int_{\mathcal{G}\setminus\mathcal{K}} |\varphi + \xi|^2\, dx + \int_{\mathcal{K}} |\varphi + \xi|^2\, dx = \int_{\mathcal{G}\setminus\mathcal{K}} |\varphi^\perp|^2\, dx + \int_{\mathcal{K}} |\varphi + \xi|^2\, dx. \tag{5.34}$$

Combining (5.33) and (5.34) we get

$$\int_{\mathcal{K}} |\varphi + \xi|^2\, dx = \int_{\mathcal{K}} |\varphi^\perp|^2\, dx + \int_{\mathcal{G}} |\chi + \xi|^2\, dx$$

and, plugging into (5.32),

$$\mathcal{L}(\varphi+\xi) \leqslant \frac{R^2}{2} - \frac{\ell^{\frac{p(2-p)}{4}}}{p} \left(\int_{\mathcal{K}} |\varphi^\perp|^2\, dx + \int_{\mathcal{G}} |\chi + \xi|^2\, dx \right)^{\frac{p}{2}} \leqslant \frac{R^2}{2} - \frac{\ell^{\frac{p(2-p)}{4}}}{p} \left(\int_{\mathcal{G}} |\chi + \xi|^2\, dx \right)^{\frac{p}{2}}. \tag{5.35}$$

Then, since χ and ξ are orthogonal by construction and $\chi+\xi$ belongs to a finite dimensional space (so that its L^2-norm is equivalent to the Y-norm), there exists $C > 0$ such that

$$\mathcal{L}(\varphi + \xi) \leqslant \frac{R^2}{2} - C \left(\|\chi\|^2 + \|\xi\|^2 \right)^{\frac{p}{2}} \leqslant \frac{R^2}{2} - C\|\xi\|^p = \frac{R^2}{2} - CR^p$$

and thus, for R large, the claim is proved.

Finally, consider the case $\mathrm{dim}V^+ < \infty$. As $\mathrm{dim}V = \infty$, we have $\mathrm{dim}V^- = \infty$. On the other hand, there holds $\sigma_2 V^- \subset Y^+$ and that $\sigma_2 V^+ \subset Y^-$, where σ_2 is the Pauli matrix

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

as this matrix anticommutes with the Dirac operator. Therefore (also recalling that σ_2 in unitary), if one defines $\widetilde{V} = \sigma_2 V$, which consists of spinors of the form.

$$\eta = \begin{pmatrix} 0 \\ \eta^2 \end{pmatrix}, \qquad \text{with} \quad \eta^2 \in C_0^\infty(I_e),$$

so that $\widetilde{V}^+ = \sigma_2 V^-$ and $\widetilde{V}^- = \sigma_2 V^+$, and then arguing as before one can easily prove

(5.28). ☐

Lemma 5.12. *There exist* $r, \rho > 0$ *such that*

$$\inf_{S_r^+} \mathcal{L} \geqslant \rho > 0,$$

where

$$S_r^+ := \left\{ \psi \in Y^+ : \|\psi\| = r \right\}. \tag{5.36}$$

Proof. The proof is an immediate consequence of the definition of $\mathcal{L}$ given in (5.22), in view of the fact that $p > 2$ and $\omega \in (-m, m)$. ☐

Finally, we mention that it will be useful in the sequel to use quantities that incorporates the frequency $\omega \in (-m, m)$. Indeed, note that as the spectrum of the (self-adjoint) operator $(\mathcal{D} - \omega)$ is given by

$$\sigma(\mathcal{D} - \omega) = (-\infty, -m - \omega] \cup [m - \omega, +\infty) \tag{5.37}$$

(and as $|\omega| < m$), one can define an equivalent norm

$$\|\psi\|_\omega := \|\sqrt{|\mathcal{D} - \omega|}\psi\|_{L^2}, \qquad \forall \psi \in Y, \tag{5.38}$$

and the two spectral projectors $P_\omega^\pm$ on the positive/negative subspace of $(\mathcal{D} - \omega)$. Then there holds:

$$\psi = P_\omega^+ \psi + P_\omega^- \psi \qquad \forall \psi \in Y. \tag{5.39}$$

As a consequence (5.27) can be also written as

$$\mathcal{L}(\psi) = \frac{1}{2}(\|\psi^+\|_\omega^2 - \|\psi^-\|_\omega^2) - \frac{1}{p}\int_{\mathcal{K}} |\psi|^p \, dx.$$

5.3.2 Existence and multiplicity of the bound states

The aim of this section is to prove, for $p > 2$, the existence of infinitely many (pairs of) bound states of the NLDE for any frequency $\omega \in (-m, m)$. The techniques used below (such as Krasnoselskij genus, pseudo-gradient flow, ...) are well-known in the literature in their abstract setting and can be found for instance in [102, 114] (see also [54] for an application to nonlinear Dirac equations).

Recall the definition of Krasnoselskij genus for the subsets of Y.

Definition. Let $\mathcal{A}$ be the family of sets $A \subset Y \backslash \{0\}$ such that A is closed and symmetric (namely, $\psi \in A \Rightarrow -\psi \in A$). For every $A \in \mathcal{A}$, the *genus* of A is the natural number defined by

$$\gamma[A] := \min\{n \in \mathbb{N} : \exists \varphi : A \to \mathbb{R}^n \backslash \{0\},\, \varphi \text{ continuous and odd}\}.$$

If no such φ exists, then one sets $\gamma[A] = \infty$.

In addition, one easily sees that the action functional $\mathcal{L}$ is even, i.e.

$$\mathcal{L}(-\psi) = \mathcal{L}(\psi), \qquad \forall \psi \in Y.$$

As a consequence, it is well known (see, e.g., [102, Appendix]) that there exists an odd pseudo-gradient flow $(h_t)_{t\in\mathbb{R}}$ associated with the functional $\mathcal{L}$, which satisfies some useful properties. This construction is based on well-known arguments and, thus, here we only present an outline of the proof, refering the reader to [102, Appendix] and [114, Chapter II] for details.

Since the interaction term is concentrated on a compact set $\mathcal{K} \subset \mathcal{G}$, the compactness of Sobolev embeddings imply that h_t can be chosen of the following form

$$h_t = \Lambda_t + K_t : [0, \infty) \times Y \longrightarrow Y,$$

where Λ_t is an isomorphism and K_t is a compact map, for all $t \geqslant 0$. Moreover, one can also prove that

$$\Lambda_t : Y^- \oplus Y^+ \longrightarrow Y^- \oplus Y^+, \qquad \forall t \in \mathbb{R},$$

that is, $Y^\pm$ are invariant under the action of Λ_t for all $t \geqslant 0$.

Fix, then, $\varepsilon > 0$ such that $\rho - \varepsilon > 0$. Exploiting suitable cut-off functions on the pseudogradient vector field, one can get that, for all $t \geqslant 0$,

$$h_t(\psi) = \psi, \qquad \forall \psi \in \{\varphi \in Y : \mathcal{L}(\varphi) < \rho - \varepsilon\}, \tag{5.40}$$

namely, the level sets of the action below $\rho - \varepsilon$ are not modified by the flow.

In view of these remarks, we can state the following lemma.

Lemma 5.13. *Let $r, \rho > 0$ be as in Lemma 5.12. Then, for every $N \in \mathbb{N}$, there results*

$$\gamma[h_t(S_r^+) \cap \mathcal{M}_N] \geqslant N, \qquad \forall t \geqslant 0, \tag{5.41}$$

with S_r^+ and $\mathcal{M}_N$ defined by (5.36) *and* (5.29)*, respectively.*

Proof. For each fixed $\psi \in Y$, the function $t \mapsto \mathcal{L} \circ h_t(\psi)$ is increasing. Then Lemma 5.11 implies that

$$h_t(S_r^+) \cap \partial\mathcal{M}_N = \emptyset, \qquad \forall t \geqslant 0.$$

Note, also, that by the group property of the pseudogradient flow

$$(h_t)^{-1} = h_{-t} = \Lambda_{-t} + K_{-t},$$

so that

$$h_t(S_r^+) \cap \mathcal{M}_N = h_t\left(S_r^+ \cap h_{-t}\left(\mathcal{M}_N\right)\right).$$

Then, a degree-theory argument (see e.g. [114, Section II.8]) shows that $S_r^+ \cap h_{-t}\left(\mathcal{M}_N\right) \neq \emptyset$.

On the other hand, by (5.40) and Lemma 5.11, it is easy to see that

$$h_t(S_r^+) \cap \mathcal{M}_N = h_t(S_r^+) \cap (Y^- \oplus Z_N),$$

and thus

$$h_t(S_r^+) \cap \mathcal{M}_N = h_t\left(S_r^+ \cap \left(Y^- \oplus Z_N' + K_{-t}(Y^- \oplus Z_N)\right)\right), \tag{5.42}$$

where $Z_N' := \Lambda_{-t}(Z_N)$ is a N-dimensional subspace of Y^+ and where we used the fact that Λ_s is an isomorphism for all $s \in \mathbb{R}$ and preserves $Y^\pm$. Now, since $h_t(0) = 0$ and $\Lambda_t(0) = 0$, we have $K_t(0) = 0$. As a consequence

$$Y^- \oplus Z_N' \subset (Y^- \oplus Z_N') + K_{-t}(Y^- \oplus Z_N),$$

and hence, exploiting (5.42) and the monotonicity of the genus,

$$\gamma\left[h_t(S_r^+) \cap \mathcal{M}_N\right] \geqslant \gamma\left[S_r^+ \cap (Y^- \oplus Z_N')\right] \geqslant \gamma\left[S_r^+ \cap Z_N'\right] = N,$$

as $S_r^+ \cap Z_N' \simeq \mathbb{S}^N$ is homeomorphic to an N-dimensional sphere. □

Lemma 5.41 has an immediate consequence, which provides the existence of the Palais-Smale sequences at the min-max levels.

Corollary 5.14. *Let the assumptions of Lemma 5.13 be satisfied and define, for any*

$N \in \mathbb{N}$,

$$\alpha_N := \inf_{X \in \mathcal{F}_N} \sup_{\psi \in X} \mathcal{L}(\psi), \tag{5.43}$$

with

$$\mathcal{F}_N := \left\{ X \in \mathcal{A} : \gamma[h_t(S_r^+) \cap X] \geqslant N, \, \forall t \geqslant 0 \right\}. \tag{5.44}$$

Then, for every $N \in \mathbb{N}$, there exists a Palais-Smale sequence $(\psi_n) \subset Y$ at level α_N, i.e.

$$\begin{cases} \mathcal{L}(\psi_n) \longrightarrow \alpha_N \\ d\mathcal{L}(\psi_n) \stackrel{Y^*}{\longrightarrow} 0, \end{cases} \qquad as \quad n \longrightarrow \infty.$$

In addition, there results

$$\alpha_{N_1} \leqslant \alpha_{N_2}, \qquad \forall N_1 < N_2, \tag{5.45}$$

$$0 < \rho \leqslant \alpha_N \leqslant \sup_{\mathcal{M}_N} \mathcal{L} < +\infty, \qquad \forall N \in \mathbb{N}.$$

Proof. The existence of a Palais-Smale sequence for $\mathcal{L}$ at level α_N follows by standard deformation arguments, and then we only sketch the proof (see [102, 114] for details).

Suppose, by contradiction, that there is no Palais-Smale sequence at level α_N. Then, since $\mathcal{L} \in C^1$, there exist $\delta, \varepsilon > 0$ such that

$$\|d\mathcal{L}(\psi)\| \geqslant \delta, \qquad \forall \psi \in \{\alpha_N - 2\varepsilon < \mathcal{L} < \alpha_N + 2\varepsilon\}. \tag{5.46}$$

In addition, from (5.43) there exists $X_\varepsilon \in \mathcal{F}_N$ such that

$$\sup_{\psi \in X_\varepsilon} \mathcal{L}(\psi) < \alpha_N + \varepsilon,$$

and hence, combining with (5.46), we can see that there exists $T > 0$ such that

$$\mathcal{L}\left(h_{-T}(X_\varepsilon)\right) \subseteq \{\mathcal{L} < \alpha_N - \varepsilon\}.$$

As a consequence, if one shows that $h_{-T}(X_\varepsilon) \in \mathcal{F}_N$, then obtains a contradiction. Note, also, that $h_{-T}(X_\varepsilon) \in \mathcal{A}$ as h_s is odd, so that it suffices to prove that

$$\gamma\left[h_t\left(S_R^+\right) \cap h_{-T}\left(X_\varepsilon\right)\right] \geqslant N.$$

First, observe that

$$h_t\left(S_r^+\right) \cap h_{-T}\left(X_\varepsilon\right) = h_{-T}\left(h_{t+T}\left(S_r^+\right) \cap X_\varepsilon\right),$$

and then the monotonicity of the genus gives

$$\gamma\left[h_t\left(S_r^+\right) \cap h_{-T}\left(X_\varepsilon\right)\right] \geqslant \gamma\left[h_{t+T}\left(S_r^+\right) \cap X_\varepsilon\right] \geqslant N.$$

Therefore, $h_{-T}(X_\varepsilon) \in \mathcal{F}_N$ and this entails that

$$\alpha_N \leqslant \sup_{\psi \in h_{-T}(X_\varepsilon)} \mathcal{L}(\psi) < \alpha_N - \varepsilon,$$

which is a contradiction.

Finally, the first line of (5.45) follows again by monotonicity of the genus, whereas the second one is a consequence of Lemma 5.12 and of the fact that $\mathcal{L}$ maps bounded sets onto bounded sets. □

Remark 5.15. It is easy to see that there are no non-trivial critical points for the action functional $\mathcal{L}$ at levels $\alpha \leqslant 0$. Indeed, let $\psi \in Y$ be such that $d\mathcal{L}(\psi) = 0$ and $\mathcal{L}(\psi) = \alpha$. A simple computation gives

$$\left(\frac{1}{2} - \frac{1}{p}\right) \int_{\mathcal{K}} |\psi|^p = \alpha.$$

This immediately implies that $\alpha \geqslant 0$. Suppose that $\alpha = 0$, then ψ must vanish on the compact core $\mathcal{K}$. By (2.49) it follows that $\psi_e^1(\mathrm{v}) = 0, \forall \mathrm{v} \in \mathcal{K}, \forall e \in E$ and thus the first equation in (5.26) implies that $\psi^1 \equiv 0$ on $\mathcal{G}$. As a consequence, since ψ satisfies a linear Dirac equation on halflines, rewriting the equation in terms of spinor components (as in (5.68),(5.69)) one sees that the second component ψ^2 must be constant and then zero, as the solution ψ is square integrable.

Now, before giving the proof of Theorem 5.6, we discuss the compactness properties of Palais-Smale sequences.

Proposition. *For every $\alpha > 0$, Palais-Smale sequences at level α are bounded in Y.*

Proof. Let (ψ_n) be a Palais-Smale sequence at level $\alpha > 0$ and assume by contradiction that, up to subsequences,

$$\|\psi_n\|_\omega \longrightarrow \infty, \qquad \text{as} \quad n \to \infty.$$

Simple computations show that, for n large,

$$\left(\frac{1}{2}-\frac{1}{p}\right)\int_{\mathcal{K}}|\psi_n|^p\,dx=\mathcal{L}(\psi_n)-\frac{1}{2}\langle d\mathcal{L}(\psi_n)|\psi_n\rangle\leqslant C+\|\psi_n\|_\omega .$$

and (recalling the definition of $P_\omega^\pm$ given by (5.39))

$$\left|\langle d\mathcal{L}(\psi_n)|P_\omega^+\psi_n\rangle\right|=\left|\int_{\mathcal{G}}\langle P_\omega^+\psi_n,(\mathcal{D}-\omega)\psi_n\rangle\,dx-\int_{\mathcal{K}}|\psi_n|^{p-2}\langle\psi_n,P_\omega^+\psi_n\rangle\,dx\right|\leqslant\|\psi_n\|_\omega .$$

As a consequence, using the Hölder inequality and (5.7), we get

$$\begin{aligned}\left|\int_{\mathcal{G}}\langle P_\omega^+\psi_n,(\mathcal{D}-\omega)\psi_n\rangle\,dx\right| &\leqslant\|\psi_n\|_\omega+\int_{\mathcal{K}}|\psi_n|^{p-1}|P_\omega^+\psi_n|\,dx\\ &\leqslant\|\psi_n\|_\omega+\left(\int_{\mathcal{K}}|\psi_n|^p\,dx\right)^{\frac{p-1}{p}}\left(\int_{\mathcal{K}}|P_\omega^+\psi_n|^p\,dx\right)^{\frac{1}{p}}\\ &\leqslant C\,(1+\|\psi_n\|_\omega)^{1-\frac{1}{p}}\,\|\psi_n\|_\omega .\end{aligned}\tag{5.47}$$

On the other hand, by the definition of $P_\omega^\pm$, one sees that

$$\|P_\omega^+\psi_n\|_\omega^2=\int_{\mathcal{G}}\langle P_\omega^+\psi_n,(\mathcal{D}-\omega)P_\omega^+\psi_n\rangle\,dx=\int_{\mathcal{G}}\langle P_\omega^+\psi_n,(\mathcal{D}-\omega)\psi_n\rangle\,dx$$

and, combining with (5.47),

$$\|P_\omega^+\psi_n\|_\omega^2\leqslant C\,(1+\|\psi_n\|_\omega)^{1-\frac{1}{p}}\,\|\psi_n\|_\omega .$$

Arguing as before, one also finds that

$$\|P_\omega^-\psi_n\|_\omega^2\leqslant C\,(1+\|\psi_n\|_\omega)^{1-\frac{1}{p}}\,\|\psi_n\|_\omega$$

and hence

$$\|\psi_n\|_\omega^2\leqslant(C+\|\psi_n\|_\omega)^{1-\frac{1}{p}}\,\|\psi_n\|_\omega ,$$

which is a contradiction if $\|\psi_n\|_\omega\to\infty$, since $1-\frac{1}{p}\in(\frac{1}{2},1)$ as $p>2$. □

Lemma 5.16. *For every $\alpha>0$, Palais-Smale sequences at level α are pre-compact in Y.*

Proof. Let (ψ_n) be a Palais-Smale sequence at level $\alpha>0$. From Proposition 5.3.2, it is bounded and then, up to subsequences,

$$\begin{aligned}&\psi_n\rightharpoonup\psi, &&\text{in}\quad Y,\\ &\psi_n\longrightarrow\psi, &&\text{in}\quad L^p(\mathcal{K},\mathbb{C}^2).\end{aligned}\tag{5.48}$$

On the other hand, by definition

$$
\begin{aligned}
o(1) &= \langle d\mathcal{L}(\psi_n) | P_\omega^+(\psi_n - \psi)\rangle \\
&= \int_{\mathcal{G}} \langle P_\omega^+(\psi_n - \psi), (\mathcal{D} - \omega)\psi_n\rangle \, dx - \int_{\mathcal{K}} |\psi_n|^{p-2} \langle \psi_n, P_\omega^+(\psi_n - \psi)\rangle \, dx,
\end{aligned} \tag{5.49}
$$

and (again) by Hölder inequality and (5.48)

$$
\begin{aligned}
\left| \int_{\mathcal{K}} |\psi_n|^{p-2} \langle \psi_n, P_\omega^+(\psi_n - \psi)\rangle \, dx \right| &\leqslant \int_{\mathcal{K}} |\psi_n|^{p-1} |P_\omega^+ \psi_n - \psi)| \, dx \\
&\leqslant \|\psi_n\|_{L^p(\mathcal{K},\mathbb{C}^2)}^{p-1} \|P_\omega^+(\psi_n - \psi)\|_{L^p(\mathcal{K},\mathbb{C}^2)} = o(1).
\end{aligned}
$$

As a consequence, combining with (5.49),

$$
\int_{\mathcal{G}} \langle P_\omega^+(\psi_n - \psi), (\mathcal{D} - \omega)\psi_n\rangle \, dx = o(1). \tag{5.50}
$$

In addition, since $(\psi_n - \psi) \rightharpoonup 0$ in Y, we get

$$
\int_{\mathcal{G}} \langle P_\omega^+(\psi_n - \psi), (\mathcal{D} - \omega)\psi\rangle \, dx = o(1)
$$

and, summing with (5.50), there results

$$
\|P_\omega^+(\psi_n - \psi)\|_\omega^2 = \int_{\mathcal{G}} \langle (\mathcal{D} - \omega) P_\omega^+(\psi_n - \psi), P_\omega^+(\psi_n - \psi)\rangle \, dx = o(1).
$$

Since, analogously, one can prove that

$$
\|P_\omega^-(\psi_n - \psi)\|_\omega^2 = \int_{\mathcal{G}} \langle (\mathcal{D} - \omega) P_\omega^-(\psi_n - \psi), P_\omega^-(\psi_n - \psi)\rangle \, dx = o(1),
$$

we obtain

$$
\|\psi_n - \psi\|_\omega^2 = o(1),
$$

which concludes the proof. $\square$

Finally, we have all the ingredients in order to prove Theorem 5.6.

Proof of Theorem 5.6. By Corollary 5.14, for every $N \in \mathbb{N}$, there exists at least a Palais-Smale sequence at level $\alpha_N > 0$ (defined by (5.43)) and, by Proposition 5.16, it converges to a critical point of $\mathcal{L}$, which is via Proposition 5.3.1 a bound state of the NLDE.

Now, if the inequalities in (5.45) are strict, then one immediately obtains the claim. However, if $\alpha_j = \alpha_{j+1} = \cdots = \alpha_{j+q}$, for some $q \geqslant 1$, then the claim follows by [13, Proposition 10.8] as the properties of the genus imply the existence of infinitely many critical points at level α_j. $\square$

5.4 Nonrelativistic limit of solutions

This section is devoted to the proof of Theorem 5.7. We prove that there exists a wide class of sequences (c_n), (ω_n) for which the nonrelativistic limit holds. More precisely, we show that with such a choice of parameters the stationary solutions of NLDE converge, as $c_n \to +\infty$, to the stationary solutions of a Schrödinger equation with the same type of nonlinearity. The strategy that we use is the one developed by M.J. Esteban and E. Séré in [50] for the case of Dirac-Fock equations. However, the differences between both the equations and the frameworks discussed call for some major modifications. In particular, while in [50] one of the main point is the estimate of the sequence of the Lagrange multipliers of bound states with fixed L^2-norm, here the major point (since there is no constraint) is to prove that the limit is non-trivial. Moreover, we also have to distinguish different cases according to the exponent $p \in (2,6)$ in the nonlinearity.

Notice that since in this section the role of the (sequence of the) speed of light is crucial, we cannot set any more $c = 1$. As a consequence, all the previous results has to be meant with m replaced by mc_n^2 (and ω replaced by ω_n). In addition, we denote by $\mathcal{D}_n$ the Dirac operator with $c = c_n$ and with $\mathcal{L}_n$ the action functional with $\mathcal{D} = \mathcal{D}_n$ and $\omega = \omega_n$. There are clearly many other quantities which depend on the index n (such as, for instance, the form domain Y, Z_N, $\dots$), but since such a dependence is not crucial we omit it for the sake of simplicity. In the following we will always make the assumptions (5.19),(5.20) and (5.21) on the parameters (c_n), (ω_n). In particular, those assumptions immediately imply that

$$0 < C_1 \leqslant mc_n^2 - \omega_n \leqslant C_2. \tag{5.51}$$

From Theorem 5.6, for every fixed $N \in \mathbb{N}$, there exist at least a pair of bound states of frequency ω_n and at level α_N^n of the NLDE at speed of light c_n. Hence, in what follows by (ψ_n) we denote a sequence of bound states corresponding to those values of parameters.

Since all the following results hold for every fixed $N \in \mathbb{N}$, the dependence on N is understood throughout (unless stated otherwise).

5.4.1 H^1-boundedness of the sequence of the bound states

The first step is to prove that the sequence (ψ_n) defined above is bounded in $L^p(\mathcal{K}, \mathbb{C}^2)$.

Lemma 5.17. *Under the assumptions* (5.19)*,* (5.20) *and* (5.21)*, the sequence* (ψ_n) *is bounded in* $L^p(\mathcal{K}, \mathbb{C}^2)$ *(uniformly with respect to* n*), as well as the associated minimax levels* (α_N^n)*.*

Proof. First, recalling (5.44) and following the notation of the proof of Lemma 5.11, one sees that

$$\alpha_N^n = \inf_{X \in \mathcal{F}_N} \sup_{\psi \in X} \mathcal{L}_n(\psi) \leqslant \sup_{Y^- \oplus Z_N} \mathcal{L}_n.$$

From, the proof of Lemma 5.11, given an orthonormal basis $\eta_j^+, j = 1, ..., N$, of Z_N, every spinor $\psi \in Y^- \oplus Z_N$ can be decomposed as

$$\psi = \varphi^\perp + \sum_{j=1}^N \lambda_j \eta_j, \qquad \lambda_1, \ldots, \lambda_N \in \mathbb{C},$$

with $\varphi^\perp \in Y^-$ orthogonal to $\zeta := \sum_{j=1}^N \lambda_j \eta_j \in V$. Arguing as in (5.31)–(5.35) we get

$$\mathcal{L}_n(\psi) \leqslant \frac{1}{2} \int_{\mathcal{G}} \langle \zeta, (\mathcal{D}_n - \omega_n)\zeta \rangle \, dx - C \left(\int_{\mathcal{G}} |\zeta|^2 \, dx \right)^{\frac{p}{2}}. \tag{5.52}$$

On the other hand, exploiting (5.30) and (5.51), there results

$$\int_{\mathcal{G}} \langle \zeta, (\mathcal{D}_n - \omega_n)\zeta \rangle \, dx = (mc_n^2 - \omega_n) \int_{\mathcal{G}} |\zeta|^2 \, dx \leqslant C \int_{\mathcal{G}} |\zeta|^2 \, dx. \tag{5.53}$$

Hence, combining (5.52) and (5.53),

$$\mathcal{L}_n(\psi) \leqslant C \int_{\mathcal{G}} |\zeta|^2 \, dx \left[1 - \left(\int_{\mathcal{G}} |\zeta|^2 \, dx \right)^{\frac{p-2}{2}} \right]$$

and thus, since V does not depend on n and since $p > 2$

$$\alpha_N^n \leqslant \max_{Y^- \oplus Z_N} \mathcal{L}_n \leqslant C < +\infty, \qquad \forall n \in \mathbb{N}.$$

Finally, as ψ_n is a critical point of the action functional,

$$\alpha_N^n = \mathcal{L}_n(\psi_n) - \frac{1}{2} \langle d\mathcal{L}_n(\psi_n), \psi_n \rangle = \left(\frac{1}{2} - \frac{1}{p} \right) \int_{\mathcal{K}} |\psi_n|^p,$$

which concludes the proof. $\square$

We can now prove that boundedness on $L^p(\mathcal{K}, \mathbb{C}^2)$ entails boundedness on $L^2(\mathcal{G}, \mathbb{C}^2)$.

Lemma 5.18. *Under the assumptions* (5.19)*,* (5.20) *and* (5.21)*, the sequence* (ψ_n) *is bounded in* $L^2(\mathcal{G}, \mathbb{C}^2)$ *(uniformly with respect to* n*).*

Proof. For the sake of simplicity, denote by $\psi^\pm$ the projections of the spinor $\psi \in Y$ given by (5.39) (with $\omega = \omega_n$). As the spectrum of the operator $\mathcal{D}_n - \omega_n$ is

$$\sigma(\mathcal{D}_n - \omega_n) = (-\infty, -mc_n^2 - \omega_n] \cup [mc_n^2 - \omega_n, +\infty) \tag{5.54}$$

and ψ_n satisfies (5.15) (with $c = c_n$ and $\omega = \omega_n$), Hölder inequality yields

$$\begin{aligned} 0 \leqslant \int_{\mathcal{G}} \langle \psi_n^+, (\mathcal{D}_n - \omega_n)\psi_n^+ \rangle \, dx = \int_{\mathcal{G}} \langle \psi_n^+, (\mathcal{D}_n - \omega_n)\psi_n \rangle \, dx \leqslant \int_{\mathcal{K}} |\psi_n|^{p-1} |\psi_n^+| \, dx \\ \leqslant \left(\int_{\mathcal{K}} |\psi_n|^p \, dx \right)^{\frac{p-1}{p}} \left(\int_{\mathcal{K}} |\psi_n^+|^p \, dx \right)^{\frac{1}{p}} \leqslant C \int_{\mathcal{K}} |\psi_n|^p \, dx \end{aligned}$$

for some $C > 0$, where in the last inequality we used the fact that the decomposition

$$Y = Y_{\omega_n}^+ \oplus Y_{\omega_n}^-$$

induces an analogous decomposition on $L^p(\mathcal{K})$, that is

$$\|\psi^\pm\|_{L^p(\mathcal{K},\mathbb{C}^2)} \leqslant C_p \|\psi\|_{L^p(\mathcal{K},\mathbb{C}^2)}, \quad \forall \psi \in Y$$

(see [43]). Moreover, using (5.54) one can prove that

$$\int_{\mathcal{G}} \langle \psi_n^+, (\mathcal{D}_n - \omega_n)\psi_n^+ \rangle \, dx \geqslant (mc_n^2 - \omega_n) \int_{\mathcal{G}} |\psi_n^+|^2 \, dx.$$

Then, combining the above observations with Lemma 5.17 and (5.51), there results

$$\|\psi_n^+\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} \leqslant M < \infty.$$

An analogous argument gives

$$(mc_n^2 + \omega_n) \|\psi_n^-\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} \leqslant M < \infty$$

and then

$$\|\psi_n^-\|_{L^2(\mathcal{G},\mathbb{C}^2)} = \mathcal{O}\left(\frac{1}{c_n}\right), \qquad \text{as} \quad n \to +\infty,$$

which concludes the proof. $\square$

Finally, we can deduce boundedness in $H^1(\mathcal{G},\mathbb{C}^2)$. Preliminarily, we recall two Gagliardo-Nirenberg inequalities for spinors that can be easily deduced from those on functions (see e.g. [112, Proposition 2.6]). For every $p \geqslant 2$, there exists $C_p > 0$ such that

$$\|\psi\|^p_{L^p(\mathcal{G},\mathbb{C}^2)} \leqslant C_p \|\psi\|^{\frac{p}{2}+1}_{L^2(\mathcal{G},\mathbb{C}^2)} \|\psi'\|^{\frac{p}{2}-1}_{L^2(\mathcal{G},\mathbb{C}^2)}, \qquad \forall \psi \in H^1(\mathcal{G},\mathbb{C}^2). \tag{5.55}$$

Moreover, there exists $C_\infty > 0$ such that

$$\|\psi\|_{L^\infty(\mathcal{G},\mathbb{C}^2)} \leqslant C_\infty \|\psi\|^{\frac{1}{2}}_{L^2(\mathcal{G},\mathbb{C}^2)} \|\psi'\|^{\frac{1}{2}}_{L^2(\mathcal{G},\mathbb{C}^2)}, \qquad \forall \psi \in H^1(\mathcal{G},\mathbb{C}^2). \tag{5.56}$$

Lemma 5.19. *Let $p \in (2,6)$. Under the assumptions* (5.19)*,* (5.20) *and* (5.21)*, the sequence (ψ_n) is bounded in $H^1(\mathcal{G},\mathbb{C}^2)$ (uniformly with respect to n).*

Proof. First, recall that, since ψ_n are bound states they satisfy (edge by edge)

$$\mathcal{D}_n \psi_n = \omega_n \psi_n + \chi_{\mathcal{K}} |\psi_n|^{p-2} \psi_n. \tag{5.57}$$

The $L^2(\mathcal{G},\mathbb{C}^2)$-norm squared of the right-hand side of (5.57) reads

$$\|\omega_n \psi_n + \kappa |\psi_n|^{p-2}\psi_n\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} = \omega_n^2 \|\psi_n\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} + \int_{\mathcal{K}} |\psi_n|^{2(p-1)}\, dx + 2\omega_n \int_{\mathcal{K}} |\psi_n|^p\, dx. \tag{5.58}$$

Let us estimate the last two integrals. Using (5.56), Lemma 5.17 and Lemma 5.18, we get

$$\begin{aligned} \int_{\mathcal{K}} |\psi_n|^{2(p-1)} &= \int_{\mathcal{K}} |\psi_n|^{p+(p-2)}\, dx \leqslant \|\psi_n\|^{p-2}_{L^\infty(\mathcal{G},\mathbb{C}^2)} \int_{\mathcal{K}} |\psi_n|^p\, dx \\ &\leqslant C_\infty^{p-2} \|\psi_n\|^{\frac{p}{2}+1}_{L^2(\mathcal{G},\mathbb{C}^2)} \|\psi_n'\|^{\frac{p}{2}-1}_{L^2(\mathcal{G},\mathbb{C}^2)} \leqslant C \|\psi_n'\|^{\frac{p}{2}-1}_{L^2(\mathcal{G},\mathbb{C}^2)}. \end{aligned} \tag{5.59}$$

On the other hand, by (5.55) and Lemma 5.18

$$\int_{\mathcal{K}} |\psi_n|^p\, dx \leqslant \int_{\mathcal{G}} |\psi_n|^p\, dx \leqslant C_p \|\psi_n\|^{\frac{p}{2}+1}_{L^2(\mathcal{G},\mathbb{C}^2)} \|\psi_n'\|^{\frac{p}{2}-1}_{L^2(\mathcal{G},\mathbb{C}^2)} \leqslant C \|\psi_n'\|^{\frac{p}{2}-1}_{L^2(\mathcal{G},\mathbb{C}^2)}. \tag{5.60}$$

Since an easy computation shows that

$$\|\mathcal{D}_n \psi_n\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} = c_n^2 \|\psi_n'\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} + m^2 c_n^4 \|\psi_n\|^2_{L^2(\mathcal{G},\mathbb{C}^2)}, \tag{5.61}$$

combining (5.61), (5.58), (5.59) and (5.60), we obtain that

$$c_n^2 \|\psi_n'\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} + m^2 c_n^4 \|\psi_n\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} \leqslant \omega_n^2 \|\psi_n\|^2_{L^2(\mathcal{G},\mathbb{C}^2)} + C(1+\omega_n) \|\psi_n'\|^{\frac{p}{2}-1}_{L^2(\mathcal{G},\mathbb{C}^2)},$$

so that, from a repeated use of (5.19) and (5.20),

$$\|\psi_n'\|_{L^2(\mathcal{G},\mathbb{C}^2)}^{\frac{6-p}{2}} \leqslant Cm.$$

Hence, the claim follows by the assumption $p < 6$. □

Remark 5.20. The above results also hold if (5.21) is replaced by the weaker assumption (5.51).

5.4.2 Passage to the limit

The last step consists in proving that the first components of the sequence of bound states (ψ_n) converges to a bound state of the NLSE, while the second component converges to zero.

For the sake of simplicity we assume throughout that the parameters p and λ are fixed and fulfill

$$p \in (2,6) \qquad \text{and} \qquad \lambda < 0.$$

In addition, we set

$$u_n := \psi_n^1 \qquad \text{and} \qquad v_n := \psi_n^2, \qquad \forall n \in \mathbb{N}, \tag{5.62}$$

and, given the two sequences (c_n) and (ω_n) introduced in the previous section (which satisfy (5.19), (5.20),(5.21) and (5.51)), we define

$$a_n := (mc_n^2 - \omega_n)b_n \qquad \text{and} \qquad b_n := \frac{mc_n^2 + \omega_n}{c_n^2}, \qquad \forall n \in \mathbb{N}. \tag{5.63}$$

Clearly, (5.51) implies that

$$b_n \longrightarrow 2m, \qquad \text{as} \quad n \to \infty \tag{5.64}$$

while (5.21) gives

$$a_n \longrightarrow -\lambda, \qquad \text{as} \quad n \to \infty. \tag{5.65}$$

We also recall that a function $w : \mathcal{G} \to \mathbb{C}$ is a bound state of the NLSE with fixed frequency λ and $\alpha = 2m$ if and only if it is a critical point of the C^2 functional $J : H \to \mathbb{R}$ defined by

$$J(w) := \frac{1}{2}\int_{\mathcal{G}} |w'|^2\,dx - \frac{2m}{p}\int_{\mathcal{K}} |w|^p\,dx - \frac{\lambda}{2}\int_{\mathcal{G}} |w|^2\,dx,$$

where

$$H := \{w \in H^1(\mathcal{G}) : (5.16) \text{ holds}\}$$

with the norm induced by $H^1(\mathcal{G})$ (this can be easily proved arguing as in [3, Proposition 3.3]). It is also worth mentioning that a Palais-Smale sequence for J is a sequence $(w_n) \subset H$ such that $dJ(w_n) \to 0$ in H^*, namely

$$\sup_{\|\phi\|_H \leqslant 1} \langle dJ(w_n)|\phi\rangle \to 0, \qquad \text{as} \quad n \to \infty.$$

Furthermore, the following property holds

Lemma 5.21. *Let (w_n) be a bounded sequence in H and, for every n, define the linear functional $A_n(w_n) : H \to \mathbb{R}$*

$$\langle A_n(w_n)|\phi\rangle := \int_{\mathcal{G}} w_n' \overline{\phi}' \, dx - b_n \int_{\mathcal{K}} |w_n|^{p-2} w_n \overline{\phi} \, dx + a_n \int_{\mathcal{G}} w_n \overline{\phi} \, dx.$$

Then, (w_n) is a Palais-Smale sequence for J if and only if

$$\sup_{\|\phi\|_H \leqslant 1} \langle A_n(w_n)|\phi\rangle \to 0, \qquad \textit{as} \quad n \to \infty. \tag{5.66}$$

Proof. The proof is trivial noting that

$$\langle A_n(w_n) - dJ(w_n)|\phi\rangle = -(b_n - m) \int_{\mathcal{K}} |w_n|^{p-2} w_n \overline{\phi} \, dx + (a_n + \lambda) \int_{\mathcal{G}} w_n \overline{\phi} \, dx$$

and exploiting (5.64), (5.65) and the fact that (w_n) is bounded in H. □

The strategy to prove Theorem 5.7 is the following:

(i) prove that the sequence (v_n) converges to 0 in $H^1(\mathcal{G})$;

(ii) prove that the sequence (u_n) is bounded away from zero in $H^1(\mathcal{G})$;

(iii) prove that the sequence (u_n) satisfies (5.66), as by Lemmas 5.19 and 5.21, this entails that it is a Palais-Smale sequence for J;

(iv) prove that the sequence (u_n) converges (up to subsequences) in H to a function u, which is then a bound state of the NLSE with frequency $\lambda < 0$.

We observe that we always tacitly use in the following the fact that, since each ψ_n is a bound state of the NLDE, then $u_n \in H$, whereas $v_n \notin H$. In addition, we highlight that, in the sequel, we often use a "formal" commutation between the differential operator

$(\cdot)'$ and $\chi_{\mathcal{K}}$. Clearly, this is just a compact notation (which avoids edious edge by edge computations) that recalls the different form of the NLDE on the bounded edges due to the presence of the localized nonlinearity.

As a first step, we prove item (i). As a byproduct of the proof, we also find an estimate of the speed of convergence of (v_n).

Lemma 5.22. *The sequence (v_n) converges to 0 in $H^1(\mathcal{G})$ as $n \to \infty$. More precisely, there holds*

$$\|v_n\|_{H^1(\mathcal{G})} = \mathcal{O}\left(\frac{1}{c_n}\right), \qquad as \quad n \to \infty. \tag{5.67}$$

Proof. As (ψ_n) is a bound state of the NLDE, rewriting the equation in terms of its components (5.62)

$$-\imath c_n v_n' + (mc_n^2 - \omega_n)u_n = \chi_{\mathcal{K}}(|u_n|^2 + |v_n|^2)^{\frac{p-2}{2}} u_n, \tag{5.68}$$

$$-\imath c_n u_n' - (mc_n^2 + \omega_n)v_n = \chi_{\mathcal{K}}(|u_n|^2 + |v_n|^2)^{\frac{p-2}{2}} v_n. \tag{5.69}$$

Dividing (5.68) by c_n and using (5.51) and Lemma 5.19, we have

$$\|v_n'\|_{L^2(\mathcal{G})} = \mathcal{O}\left(\frac{1}{c_n}\right). \tag{5.70}$$

On the other hand, dividing (5.69) by c_n^2 and using again Lemma 5.19, there results

$$\left\| -\frac{\imath}{c_n} u_n' - \frac{(mc_n^2 + \omega_n)}{c_n^2} v_n \right\|_{L^2(\mathcal{G})} = \mathcal{O}\left(\frac{1}{c_n^2}\right)$$

and hence

$$\frac{(mc_n^2 + \omega_n)}{c_n^2} \|v_n\|_{L^2(\mathcal{G})} \leqslant \left\| -\frac{\imath}{c_n} u_n' - \frac{(mc_n^2 + \omega_n)}{c_n^2} v_n \right\|_{L^2(\mathcal{G})} + \frac{1}{c_n} \|u_n'\|_{L^2(\mathcal{G})} = \mathcal{O}\left(\frac{1}{c_n}\right).$$

Finally, combining with (5.70), one obtains (5.67). □

Item (ii) requires some further effort.

Lemma 5.23. *There exists $\mu > 0$ such that*

$$\inf_{n \in \mathbb{N}} \|u_n\|_{H^1(\mathcal{G})} \geqslant \mu > 0. \tag{5.71}$$

Proof. Assume, by contradiction, that (5.71) does not hold, namely that, up to subsequences,

$$\lim_{n\to\infty} \|u_n\|_{H^1(\mathcal{G})} = 0. \tag{5.72}$$

Dividing by c_n and rearranging terms, (5.68) yields

$$-\imath v_n' = \frac{1}{c_n}\left[\chi_{\mathcal{K}}\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} + (\omega_n - mc_n^2)\right] u_n, \tag{5.73}$$

and then, using (5.51), we find

$$\int_{\mathcal{G}} |v_n'|^2\,dx \lesssim \frac{1}{c_n^2}\int_{\mathcal{G}} |u_n|^2\,dx. \tag{5.74}$$

Moreover, (5.69) can be rewritten as

$$v_n\left(1+\chi_{\mathcal{K}}\frac{\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}}}{mc_n^2+\omega_n}\right) = -\frac{\imath c_n}{mc_n^2+\omega_n}u_n' \tag{5.75}$$

and, since (again by (5.51)) $(mc_n^2+\omega_n)\sim c_n^2$, there results

$$\int_{\mathcal{G}} |v_n|^2\,dx \lesssim \frac{1}{c_n^2}\int_{\mathcal{G}} |u_n'|^2\,dx,$$

so that, combining with (5.74),

$$\|v_n\|_{H^1(\mathcal{G})} \lesssim \frac{1}{c_n}\|u_n\|_{H^1(\mathcal{G})}. \tag{5.76}$$

Note that (5.75) also shows that u_n is of class C^1 on each edge.

Now, plugging (5.75) into (5.73), one obtains

$$-u_n'' + a_n u_n = -\frac{\imath\chi_{\mathcal{K}}}{c_n}\left[\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} v_n\right]' + \chi_{\mathcal{K}} b_n\left[\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} u_n\right]. \tag{5.77}$$

Clearly, (5.77) is to be meant in a distributional sense. However, observing that it can be written as

$$-\left[u_n' - \frac{\imath\chi_{\mathcal{K}}}{c_n}\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} v_n\right]' = -a_n u_n + \chi_{\mathcal{K}} b_n\left[\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} u_n\right],$$

and that consequently the l.h.s. belongs to $L^2(\mathcal{G})$ and is continuous edge by edge (recalling also that u_n is of class C^1 edge by edge), the following multiplications by $\overline{u}_n$ and integrations (by parts) can be proved to be rigorous in the Lebesgue sense.

Therefore, multiplying (5.77) by $\overline{u}_n$ and integrating (by parts) over $\mathcal{G}$, at the l.h.s. we obtain

$$\int_{\mathcal{G}} |u_n'|^2\,dx + \underbrace{\sum_{\mathrm{v}\in\mathcal{K}}\left(\sum_{e\succ\mathrm{v}} \overline{u}_{n,e}(\mathrm{v})\frac{du_{n,e}}{dx_e}(\mathrm{v})\right)}_{\text{boundary terms}} + a_n\int_{\mathcal{G}}|u_n|^2\,dx$$

where we denote by $u_{n,e}$ (and $v_{n,e}$) the restriction of u_n (and v_n) to the edge (represented by) I_e, and $\frac{d}{dx_e}$ are to be meant as in Definition 5.2.1. Using (5.69) and the fact that u_n is of class C^1 (edge by edge), we find that

$$\begin{aligned}
&\sum_{e\succ\mathrm{v}} \overline{u}_{n,e}(\mathrm{v})\frac{du_{n,e}}{dx_e}(\mathrm{v}) = \\
&\quad = -\frac{\imath}{c_n}\sum_{e\succ\mathrm{v}}\overline{u}_{n,e}(\mathrm{v})\left((mc_n^2+\omega_n)v_{n,e}(\mathrm{v})_\pm + \left(|u_{n,e}(\mathrm{v})|^2+|v_{n,e}(\mathrm{v})|^2\right)^{\frac{p-2}{2}} v_{n,e}(\mathrm{v})_\pm\right) \\
&= \underbrace{-\frac{\imath}{c_n}\sum_{e\succ\mathrm{v}}\overline{u}_{n,e}(\mathrm{v})(mc_n^2+\omega_n)v_{n,e}(\mathrm{v})_\pm}_{=:A} - \frac{\imath}{c_n}\sum_{e\succ\mathrm{v}}\overline{u}_{n,e}(\mathrm{v})v_{n,e}(\mathrm{v})_\pm\left(|u_{n,e}(\mathrm{v})|^2+|v_{n,e}(\mathrm{v})|^2\right)^{\frac{p-2}{2}}
\end{aligned}$$

($v_{n,e}(\mathrm{v})_\pm$ meant as in Definition 2.3.2). Moreover, as u_n and v_n satisfy the vertex conditions (2.49) and (2.50) (respectively), one has

$$A = -\frac{\imath(mc_n^2+\omega_n)}{c_n}\overline{u}_n(\mathrm{v})\sum_{e\succ\mathrm{v}} v_{n,e}(\mathrm{v})_\pm = 0,$$

while, for any $\mathrm{v}\in\mathcal{K}$ and $e\succ\mathrm{v}$, there results

$$\begin{aligned}
\left|\overline{u}_{n,e}(\mathrm{v})v_{n,e}(\mathrm{v})_\pm\left(|u_{n,e}(\mathrm{v})|^2+|v_{n,e}(\mathrm{v})|^2\right)^{\frac{p-2}{2}}\right| &\leqslant \||u_n|^2+|v_n|^2\|_{L^\infty(\mathcal{G})}^{\frac{p-2}{2}}\|u_n\|_{L^\infty(\mathcal{G})}\|v_n\|_{L^\infty(\mathcal{G})} \\
&\lesssim \|u_n\|_{H^1(\mathcal{G})}\|v_n\|_{H^1(\mathcal{G})} = o\left(\|u_n\|_{H^1(\mathcal{G})}^2\right)
\end{aligned}$$

(where we used Lemma 5.19, (5.76) and Sobolev embeddings). As a consequence (since the number of the edges and the vertices is finite)

$$\sum_{\mathrm{v}\in\mathcal{K}}\left(\sum_{e\succ\mathrm{v}}\overline{u}_{n,e}(\mathrm{v})\frac{du_{n,e}}{dx_e}(\mathrm{v})\right) = o\left(\|u_n\|_{H^1(\mathcal{G})}^2\right),$$

so that (recalling (5.65))

$$\int_{\mathcal{G}} |u_n'|^2\,dx + a_n \int_{\mathcal{G}} |u_n|^2\,dx \gtrsim \|u_n\|^2_{H^1(\mathcal{G})}. \tag{5.78}$$

Let us focus on the r.h.s. of (5.77). After multiplication times $\overline{u}_n$ and integration over $\mathcal{G}$ we have

$$-\frac{\imath}{c_n}\int_{\mathcal{K}} \overline{u}_n \left[\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} v_n\right]'\,dx + b_n \int_{\mathcal{K}} \left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} |u_n|^2\,dx.$$

The latter term can be easily estimated using the Hölder inequality and (5.64), (5.72) and (5.76), i.e.

$$\begin{aligned} b_n \int_{\mathcal{K}} \left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} |u_n|^2\,dx &\lesssim \left(\|u_n\|^{p-2}_{L^\infty(\mathcal{G})} + \|v_n\|^{p-2}_{L^\infty(\mathcal{G})}\right)\int_{\mathcal{G}} |u_n|^2\,dx \\ &\lesssim \left(\|u_n\|^{p-2}_{H^1(\mathcal{G})} + \|v_n\|^{p-2}_{H^1(\mathcal{G})}\right)\|u_n\|^2_{H^1(\mathcal{G})} = o\left(\|u_n\|^2_{H^1}\right). \end{aligned}$$

On the contrary, the former one requires some further efforts. Clearly,

$$\begin{aligned} \frac{1}{c_n}\int_{\mathcal{K}} \overline{u}_n \left[\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}} v_n\right]'\,dx &= \underbrace{\frac{1}{c_n}\int_{\mathcal{K}} v_n'\overline{u}_n \left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}}\,dx}_{=:I_1} + \\ &+ \underbrace{\frac{1}{c_n}\int_{\mathcal{K}} \overline{u}_n v_n \left(|u_n|^2+|v_n|^2\right)^{\frac{p-4}{2}} \left(\overline{u}_n u_n' + \overline{v}_n v_n'\right)\,dx}_{I_2}. \end{aligned} \tag{5.79}$$

Using (5.73) and again Lemma 5.19, we immediately find that

$$|I_1| \lesssim \frac{1}{c_n^2}\|u_n\|^2_{H^1(\mathcal{G})} = o\left(\|u_n\|^2_{H^1(\mathcal{G})}\right).$$

It is, then, left to estimate I_2. We distinguish two cases.

Estimate for I_2, case $p \in (2,4)$: as $p-4<0$ there holds

$$\left(|u_n|^2+|v_n|^2\right)^{\frac{p-4}{2}} \leqslant 2^{\frac{p-4}{2}}\left(|u_n||v_n|\right)^{\frac{p-4}{2}}.$$

As a consequence

$$|I_2| \lesssim \frac{1}{c_n}\int_{\mathcal{K}} |u_n|^{\frac{p}{2}}|v_n|^{\frac{p-2}{2}}|u_n'|\,dx + \frac{1}{c_n}\int_{\mathcal{K}} |u_n|^{\frac{p-2}{2}}|v_n|^{\frac{p}{2}}|v_n'|\,dx =: I_{2,1}+I_{2,2}.$$

Moreover,

$$I_{2,1} \lesssim \frac{1}{c_n}\|v_n\|_{L^\infty(\mathcal{G})}^{\frac{p-2}{2}} \int_{\mathcal{K}} |u_n|^{\frac{p}{2}}|u_n'|\,dx$$
$$\leqslant \frac{1}{c_n}\|v_n\|_{L^\infty(\mathcal{G})}^{\frac{p-2}{2}}\|u_n\|_{L^p(\mathcal{G})}^{\frac{p}{2}}\|u_n'\|_{L^2(\mathcal{G})} \lesssim \frac{1}{c_n}\|v_n\|_{L^\infty(\mathcal{G})}^{\frac{p-2}{2}}\|u_n\|_{H^1(\mathcal{G})}^{\frac{p}{2}+1},$$

whereas

$$I_{2,2} \lesssim \frac{1}{c_n}\|u_n\|_{L^\infty}^{\frac{p-2}{2}}\|v_n\|_{H^1(\mathcal{G})}^{\frac{p}{2}+1} \lesssim \frac{1}{c_n}\|u_n\|_{L^\infty}^{\frac{p-2}{2}}\|u_n\|_{H^1(\mathcal{G})}^{\frac{p}{2}+1},$$

so that (since $p > 2$)

$$|I_2| = o\left(\|u_n\|_{H^1(\mathcal{G})}^2\right).$$

Estimate for I_2, case $p \in [4,6)$: as $p-4 \geqslant 0$, there holds

$$\left\|(|u_n|^2 + |v_n|^2)^{\frac{p-4}{2}}\right\|_{L^\infty(\mathcal{G})} \leqslant C.$$

and then arguing as before one can easily find (as well) that

$$|I_2| = o\left(\|u_n\|_{H^1(\mathcal{G})}^2\right).$$

Summing up, we proved that for all $p \in (2,6)$,there results

$$|I_1| + |I_2| = o\left(\|u_n\|_{H^1(\mathcal{G})}^2\right)$$

and hence, combining with (5.77), (5.78) and (5.79), we obtain that

$$\|u_n\|_{H^1(\mathcal{G})}^2 = o\left(\|u_n\|_{H^1(\mathcal{G})}^2\right),$$

which is the contradiction that concludes the proof. □

We now prove item (iii).

Lemma 5.24. *The sequence (u_n) is a Palais-Smale sequence for J.*

Proof. By Lemma 5.21 it is sufficient to prove (5.66). Take, then, $\varphi \in H$ with $\|\varphi\|_{H^1(\mathcal{G})} \leqslant 1$. Multiplying (5.77) by φ and integrating over $\mathcal{G}$ (which is rigorous as we showed in the proof of Lemma 5.23) one gets

$$(5.80)\quad -\int_{\mathcal{G}}\overline{\varphi}u_n''\,dx+a_n\int_{\mathcal{G}}\overline{\varphi}u_n\,dx=$$
$$=-\frac{i}{c_n}\int_{\mathcal{K}}\overline{\varphi}\left[(|u_n|^2+|v_n|^2)^{\frac{p-2}{2}}v_n\right]'\,dx+b_n\int_{\mathcal{K}}(|u_n|^2+|v_n|^2)^{\frac{p-2}{2}}u_n\overline{\varphi}\,dx.$$

Arguing as in the proof of Lemma 5.23 and using Lemma 5.22, one can check that

$$(5.81)\qquad -\int_{\mathcal{G}}\overline{\varphi}u_n''\,dx=\int_{\mathcal{G}}\overline{\varphi}_n'u_n'\,dx+\sum_{\mathrm{v}\in\mathcal{K}}\left(\sum_{e\succ\mathrm{v}}\overline{\varphi}(\mathrm{v})\frac{d}{dx}u_{n,e}(\mathrm{v})\right)=\int_{\mathcal{G}}\overline{\varphi}_n'u_n'\,dx+o(1)$$

(where throughout we mean that $o(1)$ is independent of ϕ). Now, the first integral at the r.h.s. of (5.80) reads

$$(5.82)$$
$$\int_{\mathcal{K}}\overline{\varphi}\left[(|u_n|^2+|v_n|^2)^{\frac{p-2}{2}}v_n\right]'\,dx=-\int_{\mathcal{K}}\overline{\varphi}'\left[(|u_n|^2+|v_n|^2)^{\frac{p-2}{2}}v_n\right]\,dx$$
$$+\sum_{\mathrm{v}\in\mathcal{K}}\left(\sum_{e\succ\mathrm{v}}\overline{\varphi}(\mathrm{v})(|u_{n,e}(\mathrm{v})|^2+|v_{n,e}(\mathrm{v})|^2)^{\frac{p-2}{2}}v_{n,e}(\mathrm{v})_\pm\right),$$

where the former term is estimated by

$$(5.83)\qquad \int_{\mathcal{K}}(|u_n|^2+|v_n|^2)^{\frac{p-2}{2}}|v_n||\overline{\varphi}'|\,dx\lesssim\int_{\mathcal{K}}|v_n||\varphi'|\,dx\lesssim\|v_n\|_{L^2(\mathcal{K})}\|\varphi'\|_{L^2(\mathcal{G})}=o(1),$$

whereas the latter is estimated by

$$(5.84)\quad \sum_{\mathrm{v}\in\mathcal{K}}\left(\sum_{e\succ\mathrm{v}}|\overline{\varphi}(\mathrm{v})|(|u_{n,e}(\mathrm{v})|^2+|v_{n,e}(\mathrm{v})|^2)^{\frac{p-2}{2}}|v_{n,e}(\mathrm{v})|\right)\lesssim\|\varphi\|_{L^\infty(\mathcal{G})}\|v_n\|_{L^\infty(\mathcal{G})}=o(1),$$

(exploiting Lemmas 5.19 and 5.22). It is, then, left to discuss the last term at the r.h.s. of (5.80). First note that

$$\int_{\mathcal{K}}\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}}u_n\overline{\phi}\,dx=\int_{\mathcal{K}}|u_n|^{p-2}u_n\overline{\phi}\,dx+\underbrace{\int_{\mathcal{K}}\left[\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}}-|u_n|^{p-2}\right]u_n\overline{\phi}\,dx}_{=:R}$$

and that $\left(|u_n|^2+|v_n|^2\right)^{\frac{p-2}{2}}-|u_n|^{p-2}\geqslant 0$.

Let us distinguish two cases (as in the proof of Lemma 5.23). Assume first that

$p \in (2,4)$. Therefore $0 < \frac{p-2}{2} < 1$, and this implies that

$$|R| \leqslant \int_{\mathcal{K}} [(|u_n|^2 + |v_n|^2)^{\frac{p-2}{2}} - |u_n|^{p-2}]|u_n||\overline{\varphi}|\,dx \leqslant \int_{\mathcal{K}} |v_n|^{p-2}|u_n||\overline{\varphi}|\,dx$$
$$\leqslant \|u_n\|_{L^\infty(\mathcal{G})}\|v_n\|^{p-2}_{L^\infty(\mathcal{G})}\|\overline{\varphi}\|_{L^2(\mathcal{G})} = o(1).$$

(where we used again Lemmas 5.19 and 5.22).

On the other hand, assume that $p \in (4,6)$ (the case $p = 4$ is analogous). In this case we exploit the elementary inequality

$$(a+b)^t - a^t \leqslant c_t\, b\,(a^{t-1} + b^{t-1}), \qquad \forall a, b > 0,$$

with $t > 1$ and $c_t > 0$. Then, setting $t = \frac{p-2}{2} > 1$, $a = |u_n|^2$ and $b = |v_n|^2$, we have that

$$\int_{\mathcal{K}} [\left(|u_n|^2 + |v_n|^2\right)^{\frac{p-2}{2}} - |u_n|^{p-2}]|u_n||\overline{\varphi}|\,dx \lesssim \int_{\mathcal{K}} \left(|u_n|^{\frac{p-4}{2}} + |v_n|^{\frac{p-4}{2}}\right)|v_n|^2|u_n||\phi|\,dx = o(1).$$

Summing up, we proved that for all $p \in (2,6)$ there holds

$$\int_{\mathcal{K}} \left(|u_n|^2 + |v_n|^2\right)^{\frac{p-2}{2}} u_n\overline{\varphi}\,dx = \int_{\mathcal{K}} |u_n|^{p-2}u_n\overline{\varphi}\,dx + o(1)$$

and, combining with (5.80), (5.81), (5.82), (5.83) and (5.84), one gets (5.66), which concludes the proof. □

Finally, we have all the ingredients to prove point (iv) and thus Theorem 5.7.

Proof of Theorem 5.7. From Lemma 5.24 the sequence (u_n) is a Palais-Smale sequence for J. In addition, from Lemma 5.19 it is bounded in H so that (up to subsequences)

$$\begin{cases} u_n \rightharpoonup u & \text{in} \quad H^1(\mathcal{G}), \\ u_n \to u & \text{in} \quad L^p(\mathcal{K}). \end{cases} \tag{5.85}$$

Now, following [111], define the linear functional $B(u) : H^1(\mathcal{G}) \to \mathbb{R}$

$$B(u)v := \int_{\mathcal{G}} u'\overline{v}'\,dx - \lambda \int_{\mathcal{G}} u\overline{v}\,dx.$$

From Lemma 5.24, (5.64), (5.65) and (5.85),

$$
\begin{aligned}
o(1) &= \langle A_n(u_n) - B(u) | u_n - u \rangle \\
&= \int_{\mathcal{G}} |u_n' - u'|^2 \, dx - b_n \int_{\mathcal{K}} |u_n|^{p-2} u_n (\overline{u}_n - \overline{u}) \, dx + a_n \int_{\mathcal{G}} u_n (\overline{u}_n - \overline{u}) \, dx + \lambda \int_{\mathcal{G}} u (\overline{u}_n - \overline{u}) \, dx = \\
&= \int_{\mathcal{G}} |u_n' - u'|^2 \, dx - \lambda \int_{\mathcal{G}} |u_n - u|^2 \, dx + o(1),
\end{aligned}
$$

and, since $\lambda < 0$, this entails that $u_n \to u$ in $H^1(\mathcal{G})$. Since by Lemma 5.23 $u \neq 0$ (recalling also Lemma 5.22), the claim of the theorem is proved. $\square$

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Résumé

Ces dernières années, de nouveaux matériaux bidimensionnels aux propriétés surprenantes ont été découverts, le plus connu étant le graphène. Dans ces matériaux, les électrons du niveau de Fermi ont une masse apparente nulle, et peuvent être décrits par l'équation de Dirac sans masse. Un tel phénomène apparaît dans des situations très générales, pour les matériaux bidimensionnels ayant une structure périodique en "nid d'abeille". La prise en compte d'interactions mène à des équations non linéaires, qui apparaissent également dans l'étude des paquets d'ondes lumineuses dans certaines fibres optiques.

Le but de cette thèse est d'étudier l'existence et la multiplicité de solutions stationnaires de ces équations avec termes non linéaires sous-critiques et critiques. Du point de vue mathématique, on doit résoudre les équations d'Euler-Lagrange de fonctionnelles d'énergie fortement indéfinies faisant intervenir l'opérateur de Dirac. Il s'agit en particulier d'étudier le cas des non-linéarités avec exposant critique, encore mal comprises pour ce type de fonctionnelle, et qui apparaissent naturellement en optique non linéaire.

Mots Clés

graphène, équation de Dirac non linéaire, méthodes variationnelles, solutions stationnaires, graphes quantiques, cones de Dirac.

Abstract

Recently new two dimensional material possessing surprising properties have been discovered, the most famous being graphene. In this materials, electrons at the Fermi level can be described by a massless Dirac equations. This holds true, more generally, for two dimensional honeycomb structures, under fairly general hypothesis. Taking into account interactions naturally leads to nonlinear Dirac equations, which also appear in the description of the propagation of light pulses in optical fibers.

The aim of this thesis is to investigate existence and multiplicity properties of stationary solutions to subcritical and critical Dirac equations, which arise as Euler-Lagrange equations of strongly indefinite functionals involving the Dirac operator. We have to deal with the case of critical nonlinearities, still poorly understood (at least in the low dimensional case), and which appear naturally in nonlinear optics.

Keywords

graphene, nonlinear Dirac equations, variational methods, stationary solutions, quantum graphs, Dirac materials.