

# Graphs, hybrids and something else

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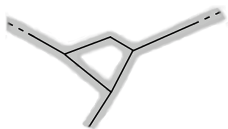


Dipartimento di Matematica ed Applicazioni R.Caccioppoli

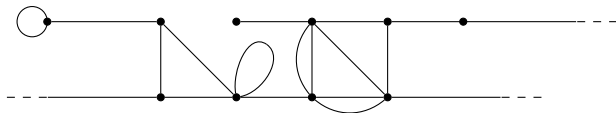
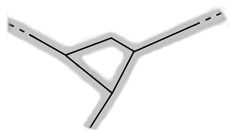
Research Team: A. Mercaldo, M.R. Posteraro

Naples – 20/10/2021

# Quantum graphs

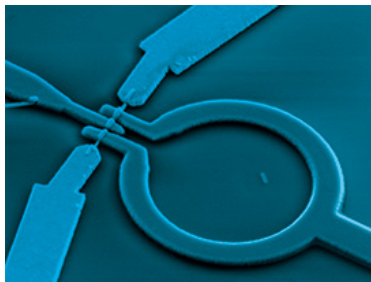
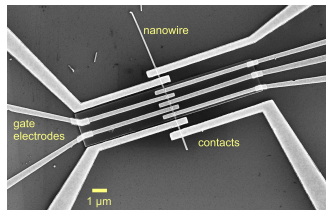


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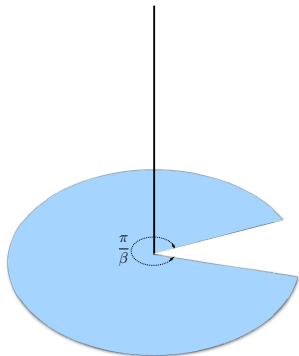


19 edges (2 self-loops, 2 multiple, 3 unbounded),  
13 vertices (1 of degree two, 3 at infinity).

# Quantum hybrids



# Quantum hybrids



## Standard NLS

The **standard** nonlinear Schrödinger equation (a.k.a. **NLS**) is

$$i \frac{\partial \psi}{\partial t} = -\Delta \psi + \beta |\psi|^{2\sigma} \psi,$$

with  $\psi(t, \mathbf{x}) : \mathbb{R}^+ \times \mathbb{R}^d \rightarrow \mathbb{C}$ ,  $\beta \in \mathbb{R}$  and  $\sigma > 0$ .

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Applications:

- (i) **laser beams:** e.g. [Rasmussen, Rypdal, Phys. Scr. '86];
- (ii) **Bose-Einstein condensates** (a.k.a. **BEC**): e.g. [Dalfovo, Giorgini, Pitaevskii, Stringari, RevModPhys '99];
- (iii) **other applications:** e.g. [Malomed, '05]:
  - ↪ nonlinear optics, plasma waves, FitzHugh-Nazumo model,...



## Effective equation

A system of  $N$  quantum particles with positions  $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^3$  is described by a wave function  $\Psi(t, \mathbf{x}_1, \dots, \mathbf{x}_N)$  that satisfies

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Kinetic energy  
of the particles

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Two-body interaction  
potential

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Scaling factors connected  
to the energy of the interactions

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For a wide class of  $V$  and for suitable  $a(\cdot)$  and  $b(\cdot)$  and for large  $N$ ,

$$\Psi(t, \mathbf{x}_1, \dots, \mathbf{x}_N) \rightsquigarrow \psi(t, \mathbf{x}_1) \dots \psi(t, \mathbf{x}_N)$$

with  $\psi$  satisfying the NLS (with  $\sigma = 1$ ):

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For a wide class of  $V$  and for suitable  $a(\cdot)$  and  $b(\cdot)$  and for **large**  $N$ ,

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Hot topic in mathematical physics:

$\rightsquigarrow$  Adami, Bardos, Brennecke, Erdos, Frank Golse, Lewin, Lieb, Loss, Paul, Pickl, Rodnianski, Rougerie, Schlein, Seiringer, Solovej, Spohn, Teta, Teufel, Yau, Yngvason...

## Concentrated nonlinearity

### Question:

↪ what if the particles are **forced** (e.g., by a confining potential) to **concentrate in a region small** with respect to the wavelength of the particles? Which is the best **effective model**?



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## Applications:

- (i) **Solid state physics:** charge accumulation in semiconductors in presence of an impurity;
  - (ii) **Nonlinear optics:** propagation in presence of localized defects.
- ↪ [Jona-Lasinio et al., PRB '91], [Malomed, Azbel, PRB '93], [Jona-Lasinio et al., APHY '95], [Bulashenko et al., PRB '96], [Sukhorukov et al., PRE '99] ...

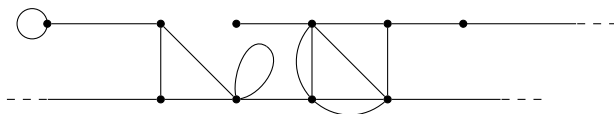
# Nonlinear Dirac equation on graphs with localized nonlinearities: bound states and nonrelativistic limit

## Notation

A **metric graph** is a graph  $\mathcal{G} := (V, E)$  s.t.:

- i)  $\mathcal{G}$  is a **multigraph** (i.e., self-loops, multiple edges, etc...);
- ii) each edge  $e \in E$  is associated with  $l_e = [0, \ell_e]$ , if **bounded**, or with  $l_e = [0, \infty)$ , if unbounded (a **half-line**).

References: [Exner, Keating, Kuchment, Sunada, Teplyaev, '08], [Post, '12], [Berkolaiko, Kuchment, '13].



19 edges (2 self-loops, 2 multiple, 3 unbounded),  
13 vertices (1 of degree two, 3 at infinity).

Note: for **bounded** edges the **orientation** of the parametrization  $x_e \in l_e$  is **free**, while for **half-lines** vertices at **infinity** correspond to  $x_e = +\infty$ .

# Notation

Further assumptions:

- i) the **cardinality** of  $V$  and  $E$  is **finite**  $\rightsquigarrow$  **no periodic graphs!**;
- ii)  $\mathcal{G}$  is **connected** (a path between each pair of vertices);
- iii)  $\mathcal{G}$  is **noncompact**  $\rightsquigarrow$  from i) this entails at least a **half-line**.

As usual, a function  $u : \mathcal{G} \rightarrow \mathbb{C}$  is a **family** of functions  $u = (u_e)_{e \in E}$ , with  $u_e := u|_{I_e} : I_e \rightarrow \mathbb{C}$ . As a consequence,

Lebesgue:  $L^p(\mathcal{G}) := \bigoplus_{e \in E} L^p(I_e) \rightsquigarrow \|u\|_{L^p(\mathcal{G})}^p := \|u_e\|_{L^p(I_e)}^p$

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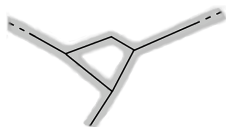
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Note: usually in the definition of  $H^1(\mathcal{G})$  there is also a **global continuity**

**condition**; for our purposes it is better to keep this condition **separated**.

# Motivation

Supposed to be good approximations for constrained dynamics in which transversal dimensions are small with respect to longitudinal ones.



Topical example: **NonLinear Schrödinger Equation (NLSE)**.

↪ Effective model for **Bose-Einstein** Condensates (BEC) in **ramified traps**, for nonlinear **optical fibers**, etc...

Literature:

↪ [Gnutzmann, Smilanski, AdvPhys '06]

↪ [Noja, RSTA '14], [Adami, Serra, Tilli, RivMatUnivParma '17]

↪ [Lorenzo et al., PHYSLETA '14]

## NLSE with Kirchhoff conditions

The **focusing** (NLSE) on metric graphs with homogeneous **Kirchhoff** vertex conditions reads:

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# Bound states of the NLSE

Problem: existence of **bound states (B.S.)**, i.e.  $L^2$ -solutions of the form

$$\psi(t, x) := e^{-i\lambda t} u(x), \quad \lambda \in \mathbb{R}.$$

Definition – B.S. of the NLSE

A **bound state** of the (NLSE) is a function  $u \neq 0$  s.t.  $u \in \text{dom}(-\Delta)$  and there exists  $\lambda \in \mathbb{R}$  s.t.

$$-u_e'' - |u_e|^{p-2} u_e = \lambda u_e, \quad \forall e \in E.$$

Literature:

- i) **real line:** e.g. [Zakharov, Shabat, JETP '72], [Cazenave, Lions, CMP '82];
- ii) **infinite N-star:** e.g. [Adami, Cacciapuoti, Finco, Noja, JPA '12 - JDE '14 - ANIHPC '14], [Kairzhan, Pelinovsky, JPA '18 - JDE '18];
- ii) **tadpole:** e.g. [Cacciapuoti, Finco, Noja, PhysRevE '15], [Noja, Pelinovsky, Shaikhova, Nonlin '15];
- iv) **general:** e.g. [Adami, Serra, Tilli, CVPDE '15 - JFA '16 - CMP '17 - arXiv '17].

## Localized nonlinearity

### Definition – Compact core

The **compact core** of  $\mathcal{G}$ , denoted by  $\mathcal{K}$ , is the metric subgraph of  $\mathcal{G}$  consisting of all its **bounded** edges.

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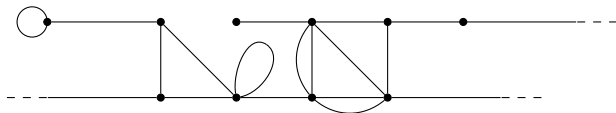
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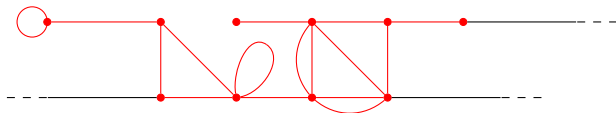


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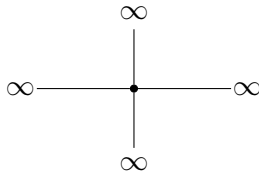


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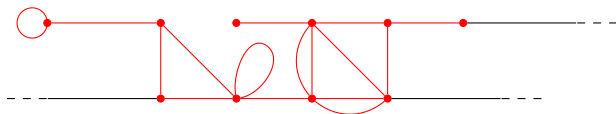


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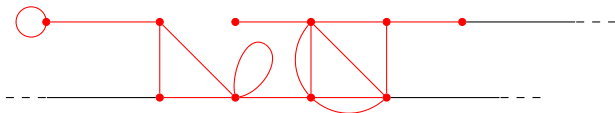
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## Definition – B.S. of the NLSE with Localized Nonlinearity

A **bound state** of the (NLSE) with **Localized Nonlinearity (L.N.)** is a function  $u \neq 0$  s.t.  $u \in \text{dom}(-\Delta)$  and there exists  $\lambda \in \mathbb{R}$  s.t.

$$-u_e'' - \chi_{\mathcal{K}} |u_e|^{p-2} u_e = \lambda u_e, \quad \forall e \in E.$$

## B.S. with Localized Nonlinearity

1. [Tentarelli, JMAA '16]:

↪ Existence/nonexistence of constrained minimizers of

$$\mathcal{E}_{\mathcal{K}}(v) := \frac{1}{2} \int_{\mathcal{G}} |v'|^2 dx - \frac{1}{p} \int_{\mathcal{K}} |v|^p dx,$$

on  $\{\|v\|_L^2(\mathcal{G}) = \mu > 0\}$ , in the  $L^2$ -subcritical case  $p \in (2, 6)$ .

2. [Serra, Tentarelli, JDE '16], [Serra, Tentarelli, NA '16]:

↪ Existence/nonexistence (respectively) of constrained critical points of the functional  $\mathcal{E}_{\mathcal{K}}(\cdot)$  (in the  $L^2$ -subcritical case).

3. [Dovetta, Tentarelli, arXiv '18]:

↪ Existence/nonexistence of constrained minimizers of  $\mathcal{E}_{\mathcal{K}}(\cdot)$  in the  $L^2$ -critical case  $p = 6$  (for a tadpole graph);  
↪ Ongoing project.

# B.S. with Localized Nonlinearity

	Exponents	Ground	Bound
NLSE	$p \in (2, 4)$	- yes, $\forall \mu > 0$	(see box below)
	$p \in [4, 6)$	- yes if $\mu > \mu_1$ - no if $\mu < \mu_2$ - unknown if $\mu \in [\mu_2, \mu_1]$	- yes (and multiple) if $\mu$ is large enough - yes if $\mathcal{G}$ has a loop or two terminal edges - no (with $\lambda \leq 0$ ) if $\mu < (p/2)^{2/(2-p)} \mu_2$ - no (with $\lambda \geq 0$ ) if $\mathcal{G}$ has (at most) one terminal edge and no loops - unknown otherwise
	$p = 6$	- yes if $\mu \in [\mu_{\mathcal{K}}, \mu_{\mathbb{R}}]$ and if no terminal edges and no cycle coverings* - no otherwise	- yes if $\mathcal{G}$ has a loop or two terminal edges - no (with $\lambda \geq 0$ ) if $\mathcal{G}$ has (at most) one terminal edge and no loops - unknown otherwise
	$p > 6$	- unknown	(see box above)

# From Schrödinger to Dirac

Recently, [Sabirov, Babajanov, Matrasulov, Kevrekidis, arXiv '17] proposed the study of the **NonLinear Dirac Equation (NLDE)**

$$i \frac{\partial \Psi}{\partial t} = \mathcal{D} \Psi - |\Psi|^{p-2} \Psi \quad \text{on } \mathcal{G} \quad (p \geq 2), \quad (\text{NLDE})$$

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

Applications: take into account **relativistic effects**.

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# Spinors on metric graphs

Since  $\mathcal{D}$  is a **matricial operator**, the first difference with (NLSE) is that (NLDE) has a **spinorial nature**; namely the unknown is a **2-spinor**:

$$\psi = (\psi_e) = \begin{pmatrix} \varphi \\ \eta \end{pmatrix} : \mathcal{G} \longrightarrow \mathbb{C}^2$$

where  $\varphi = (\varphi_e)$ ,  $\eta = (\eta_e)$  are **functions on graphs**.

Lebesgue:  $L^p(\mathcal{G}, \mathbb{C}^2) := \{\varphi, \eta \in L^p(\mathcal{G})\}$

$$\rightsquigarrow \|\psi\|_{L^p(\mathcal{G}, \mathbb{C}^2)}^p := \|\varphi\|_{L^p(\mathcal{G})}^p + \|\eta\|_{L^p(\mathcal{G})}^p,$$

Sobolev:  $H^1(\mathcal{G}, \mathbb{C}^2) := \{\varphi, \eta \in H^1(\mathcal{G})\}$

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

However,  $\mathcal{D}$  is just **formal** since it is **not defined** at the vertices! ...

## Kirchhoff-type vertex conditions

To find a suitable s.a. realization of  $\mathcal{D}$

We choose the following:

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

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$$\varphi_{e_1}(v) = \varphi_{e_2}(v), \quad \forall e_1, e_2 \succ v, \quad \forall v \in V \setminus V_\infty \quad (\text{KT1})$$

$$\sum_{e \succ v} \eta_e(v)_\pm = 0, \quad \forall v \in V \setminus V_\infty \quad (\text{KT2})$$

# Kirchhoff-type vertex conditions

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$$\mathcal{D}\psi|_{l_e} = \mathcal{D}_e\psi_e := -i c \sigma_1 \psi'_e + m c^2 \sigma_3 \psi_e, \quad \forall e \in E, \quad \forall \psi \in \text{dom}(\mathcal{D}),$$

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$\eta_e(v)_\pm$  stands for  $\eta_e(0)$  or  $-\eta_e(\ell_e)$  depending on the **orientation** of  $l_e$ .



## Kirchhoff-type vertex conditions

One can check (using [Bulla, Trenkler, JMP '90], [Bolte, Harrison, JPA '03],[Post, '08], [C., Malamud, Posilicano, JDE '13]) that:

- i)  $\mathcal{D}$  is **self-adjoint**;
- ii) the spectrum is absolutely continuous and presents a **gap**, i.e.

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

We call (KT1)-(KT2) Kirchhoff-type vertex conditions.

### Why?

1. They identify (as Kirchhoff for  $-\Delta$ ) the **free case**: **no effect** at the vertices (which are then **mere junctions** between the edges).

↪ Introduced by [Sabirov, Babajanov, Matrasulov, Kevrekidis, arXiv '17]

(where are derived by some **conservation laws**).

2. They converge to the Kirchhoff ones in the **nonrelativistic limit**.

# Quadratic form

Formally, the **quadratic form** associated with  $\mathcal{D}$  should read

$$\mathcal{Q}(\psi) := (\psi, \mathcal{D}\psi)_{L^2(\mathcal{G}, \mathbb{C}^2)} = \frac{1}{2} \int_{\mathcal{G}} \psi \cdot \mathcal{D}\psi \, dx,$$

with domain  $H^{1/2}(\mathcal{G}, \mathbb{C}^2) := \{\varphi, \eta \in H^{1/2}(\mathcal{G})\}$ .

- i) the derivative of a function in  $H^{1/2}(I_e)$  belongs to  $H^{-1/2}(I_e)$ , which is **not the dual** of  $H^{1/2}(I_e)$  if  $I_e$  is **bounded**;
- ii)  $H^{1/2}(I_e) \not\leftrightarrow C^0(I_e) \Rightarrow$  **cannot “just add”** a boundary condition

$\rightsquigarrow$  as for  $-\Delta$ , where the definitions of the quadratic form and its domain are immediate, i.e.

$$\frac{1}{2} \|v'\|_{L^2(\mathcal{G})}^2, \quad \text{with domain } H^1(\mathcal{G}) \text{ “+” (K1).}$$

Problem: how to define  $\mathcal{Q}$  and  $\text{dom}(\mathcal{Q})$ ?

## Quadratic form

↪ There exists  $U$  **unitary** that transforms  $\mathcal{D}$  into a **multiplication operator**  $f$  on  $L^2(M, d\mu)$ .

↪ Hence,  $\mathcal{Q}(v) := \frac{1}{2}(Uv, f Uv)_{L^2(M, d\mu)}$  and

$$\text{dom}(\mathcal{Q}) := \{ \|\sqrt{|f|} Uv\|_{L^2(M, d\mu)} < \infty \}.$$

This could seem quite **abstract**, but, by standard **Interpolation Theory**,

$$\text{dom}(\mathcal{Q}) = [L^2(\mathcal{G}), \text{dom}(\mathcal{D})]_{\frac{1}{2}}$$

and

$$H^{1/2}(\mathcal{G}, \mathbb{C}^2) = [L^2(\mathcal{G}), H^1(\mathcal{G}, \mathbb{C}^2)]_{\frac{1}{2}},$$

$$\text{dom}(\mathcal{Q}) \hookrightarrow H^{1/2}(\mathcal{G}, \mathbb{C}^2) \hookrightarrow L^p(\mathcal{G}, \mathbb{C}^2) \quad (2 \leq p < \infty).$$

## Back to nonlinear

Now, we have a precise meaning for (NLDE)

$$i \frac{\partial \Psi}{\partial t} = \mathcal{D}\Psi - |\Psi|^{p-2}\Psi$$

where  $\mathcal{D}$  is the **Dirac** operator with **Kirchhoff-type** vertex conditions.

Goal: **bound states**, that is solutions of the form

$$\Psi(t, x) := e^{-i\omega t} \psi(x), \quad \omega \in \mathbb{R}.$$

Problem: we **cannot** search for **constrained minimizers** since, the associated

$$\mathcal{E}(\psi) := \mathcal{Q}(\psi) - \frac{1}{p} \int_{\mathcal{G}} |\psi|^p dx$$

is **unbounded below**, even if one **fixes the  $L^2$ -norm**

↪ due to the **spectral** properties of  $\mathcal{D}$ , precisely to the presence of an **infinite negative** portion of the **spectrum**.

## Main results: B.S. with localized nonlinearities

In addition, we decided to first study the case of the **localized nonlinearity**; that is, to search for

Definition – B.S. of the NLDE with L.N.

A **B.S.** of the (NLDE) with **L.N.** is a spinor  $\psi \neq 0$  s.t.:

- i)  $\psi \in \text{dom}(\mathcal{D})$ ;
- ii) there exists  $\omega \in \mathbb{R}$  s.t.

$$\mathcal{D}_e \psi_e - \chi_{\mathcal{K}} |\psi_e|^{p-2} \psi_e = \omega \psi_e, \quad \forall e \in E.$$

Then, we proved:

Theorem 1 [T.B.C., SIMA '19]

Let  $\mathcal{K} \neq \emptyset$  and let  $p > 2$ . Then, for every  $\omega \in (-mc^2, mc^2) = \mathbb{R} \setminus \sigma(\mathcal{D})$ , there exists **infinitely many** (distinct pairs of) **B.S.** of frequency  $\omega$  of the (NLDE) with **L.N.**.

## Main results: nonrelativistic limit

By the definition of  $\mathcal{D}$ , the B.S. obtained via Theorem 1 depend on the relativistic parameter  $c$  (the mass  $m$ ) and the frequency  $\omega$ :

$\rightsquigarrow$  meant as B.S. at (a fixed value) speed of light  $c$  and frequency  $\omega$ .

Theorem 2 [T.B.C., SIMA'19]

Let  $\mathcal{K} \neq \emptyset$ ,  $p \in (2, 6)$  and  $\lambda < 0$ . Let also  $(c_n)$  and  $(\omega_n)$  be two real sequences such that

$$0 < c_n, \omega_n \rightarrow \infty, \quad \omega_n < mc_n^2, \quad \omega_n - mc_n^2 \rightarrow \frac{\lambda}{m}.$$

If  $\{\psi_n = (\varphi_n, \eta_n)^T\}$  is a sequence of B.S. of frequency  $\omega_n$  of the (NLDE)

with L.N. at speed of light  $c_n$ ,

$$\varphi_n \rightarrow u \quad \text{and} \quad \eta_n \rightarrow 0 \quad \text{in} \quad H^1(\mathcal{G}),$$

where  $u$  is a B.S. of frequency  $\lambda$  of the (NLSE) with L.N.

## B.S. EXISTENCE

1. First **variational** result on the B.S. of the **(NLDE)** on metric graphs.
2. **Differences** with respect to the **(NLSE)** on graphs:
  - i) one cannot search for **constrained minimizers** of a proper **energy** functional, since the **kinetic** part  $Q$  is **unbounded from below**;
  - ii) one cannot use the adaptations of **direct methods** of **calculus of variations** introduced for the **(NLSE)**;
  - iii)  $Q$  is **strongly indefinite** in sign:
    - $\rightsquigarrow$  more refined tools of **Critical Point Theory**;
    - $\rightsquigarrow$  more **complex geometry** of the functional (**linking**);
  - iv) the **spinorial nature** and the **implicit definition** of  $Q$ :
    - $\rightsquigarrow$  one cannot use of the techniques of **rearrangements** and “**graph surgery**” developed for **(NLSE)**.

## Remarks

3. It is necessary to adapt **classical techniques** for (NLDE) on **standard** domains (e.g. [Rabinowitz, '80], [Esteban, Séré, CMP '95], [Struwe, '08]).

### NONRELATIVISTIC LIMIT

1. Actually, the B.S. converge to the (NLSE) with a **pre-factor**  $2m$  in front of the nonlinearity.
2. Theorem 2 holds just in the  **$L^2$ -subcritical case**  $p \in (2, 6)$ .
3. As a byproduct, Theorem 2 is an **existence** result for the (NLSE) **parametrized** by  $\lambda$  and not by  $L^2$ -norm.
4. The meaning of the **nonrelativistic limit** is to investigate what occurs when the **relativistic** effects become **negligible** (i.e.  $c_n \rightarrow \infty$ ):
  - $\rightsquigarrow$  the convergence to (NLSE) is a **rigorous** justification of the **physical** intuition.
  - $\rightsquigarrow$  also justifies **Kirchhoff-type** vertex conditions.