Qualitative properties of solutions of the nonlinear Schrödinger equation on metric graphs (II)

Graduate Lecture Series in Analysis and PDEs, Brown University

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Joint work with Colette De Coster (CERAMATHS/DMATHS, Valenciennes, France) and Christophe Troestler (UMONS, Mons, Belgium)

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- you!

A first example

Let us compute $\sin(0)$ and $\sin(\pi)$ using Python.

Image from `https://fr.wikipedia.org/wiki/Fichier:Python-logo-notext.svg`

Floating-point numbers in a nutshell

Rough idea

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$\mathbb{F}$: set of finite 64 bit (double precision) floating-point numbers.

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- there is not a well-defined total order!
- etc.

How not to launch a rocket

Figure: An Ariane 5 launcher (click for the video)

Image from https://commons.wikimedia.org/wiki/File:Ariane_5_with_James_Webb_Space_Telescope_Prelaunch_(51773093465).jpg,

video from https://www.youtube.com/watch?v=1qRUFg-Pte0

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To summarize:

A first (obvious) limitation of numerical computations

$\mathbb{F}$ is **finite**!

Rounding modes

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There are thus several *rounding modes*, depending on whether the result is to be rounded up, down, towards zero, etc.

Accumulation of round-off errors

The Vancouver stock index

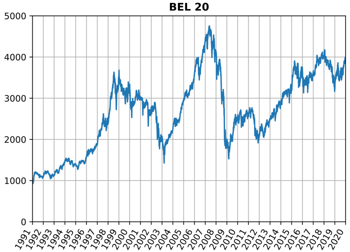

Figure: The BEL20 stock index

Image from `https://commons.wikimedia.org/wiki/File:BEL_20.svg`

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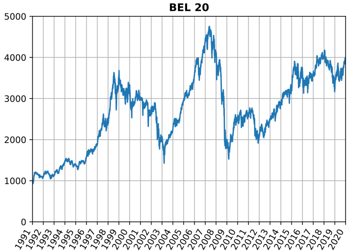
The Vancouver stock index

Between 1982 and 1983, the Vancouver stock index dropped anomalously due to the accumulation of small round-off errors, due to the fact that quantities were always rounded *down* after each computation.



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Patriot missiles

Figure: A Patriot missile launch

Image from

https://upload.wikimedia.org/wikipedia/commons/f/f8/Patriot_missile_launch_b.jpg

Accumulation of round-off errors
Patriot missiles

In 1991, American Patriot missiles failed to intercept an incoming Scud missile, killing 28 soldiers and injuring 100 other people, due to a bad computation of internal time due to an accumulation of round-off errors.

Figure: A Patriot missile launch

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Approximation errors are typically studied by numerical analysts: rigorous error bounds, convergence results, etc.

As for round-off errors, in "practical applications" it is important to **be aware** of them and to **keep them small by design**. This typically involves a suitable **stability analysis** of the numerical methods.

Where are we now?

For us, an important question remains.

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How to obtain **mathematically rigorous** results based on numerical computations?

If only one could ignore round-off errors...

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- to physicists: physical measurements are performed up to a finite precision anyway.

Although this may seem a paradox, all exact science is dominated by the idea of approximation.

— Bertrand Russell, The Scientific Outlook

The class $\mathcal{I}_{\mathbb{R}}$ of intervals

The intervals we will consider are the topologically closed and connected subsets of $\mathbb{R}$ (as specified in the standard IEEE-1788 devoted to interval arithmetic[1]), i.e. they belong to the class $\mathcal{I}_{\mathbb{R}}$ of subsets of $\mathbb{R}$ defined by

$$\begin{aligned}\mathcal{I}_{\mathbb{R}} := \left\{\emptyset\right\} &\cup \left\{[a,b] \mid a,b \in \mathbb{R}, a \leq b\right\}\\ &\cup \left\{[a,+\infty[\mid a \in \mathbb{R}\right\}\\ &\cup \left\{]-\infty,b] \mid b \in \mathbb{R}\right\}\\ &\cup \left\{]-\infty,+\infty[:= \mathbb{R}\right\}.\end{aligned}$$

[1] See `https://standards.ieee.org/ieee/1788/4431/`.

Operations on intervals

Given two intervals **x** and **y**, their *sum* is given by

$$\mathbf{x} + \mathbf{y} := \left\{ x + y \mid x \in \mathbf{x}, y \in \mathbf{y} \right\},$$

their *difference* by

$$\mathbf{x} - \mathbf{y} := \left\{ x - y \mid x \in \mathbf{x}, y \in \mathbf{y} \right\}$$

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Examples and surprises: on the blackboard!

In general: interval extensions

Definition

Let $D \subseteq \mathbb{R}$ be a set and let $F : D \to \mathbb{R}$ be a map.

An *interval extension* of F is an application $\mathbf{F} : \mathcal{I}_{\mathbb{R}} \to \mathcal{I}_{\mathbb{R}}$ which satisfies the *containment property*, namely so that for all $\mathbf{x} \in \mathcal{I}_{\mathbb{R}}$, the set

$$F(\mathbf{x}) := \left\{ F(x) \mid x \in \mathbf{x} \cap D \right\}$$

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Examples on the blackboard! *Compare extensions of* $F : \mathbb{R} \to \mathbb{R} : x \mapsto x^2$ *with the product operation.*

Fundamental theorem of interval arithmetic

Theorem

If interval extensions of real functions $f_1, \dots, f_k$ are composed, the result is an interval extension of the composition $f_1 \circ \cdots \circ f_k$.

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Allows to obtain interval extensions of complicated functions by composing interval extensions of its subparts.

In practice

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In practice, the implementation will use intervals from the set

$$\mathcal{I}_{\mathbb{F}} := \left\{ \mathbf{x} = [\underline{x}, \overline{x}] \mid \underline{x} \leq \overline{x} \text{ are two floating-point numbers} \right\} \cup \left\{ \emptyset \right\}.$$

Back to the computation of sin(π)

Let us use the "`mpmath`" library[2] in Python3 and ask the value of

```
iv.pi
```

then

```
iv.sin(iv.pi).
```

[2]See in particular the module `iv`, devoted to interval arithmetic at `https://www.mpmath.org/doc/1.0.0/contexts.html`.

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- If a returned interval is “too big”, it is valid but useless.
  For instance, `iv.sin(x)` could return `[-1, 1]` regardless of the value of `x`, but this bound is useless.
- Nevertheless, it is in principle possible to show that given matrices are invertible, positive/negative definite... using interval arithmetic.

Locating roots of a function

Let $F : [0, 1] \to \mathbb{R}$. If $\mathbf{F}$ is an interval extension of F and if $\mathbf{x} \in \mathcal{I}_{\mathbb{R}}$ is included in $[0, 1]$, then

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We may thus divide $[0, 1]$ into many “small” intervals and discard all those for which we are sure that F has no roots, this being determined by evaluating the interval extension $\mathbf{F}$. We end up with (possibly many) small intervals such that all potential roots of F belong to one of those.

Application of interval arithmetic to nonlinear analysis

Existence of the Lorenz strange attractor

The system of ODEs

$$\begin{aligned} \partial_t x_1 &= -\sigma x_1 + \sigma x_2 \\ \partial_t x_2 &= \rho x_1 - x_2 - x_1 x_3, \\ \partial_t x_3 &= -\beta x_3 + x_1 x_2 \end{aligned}$$

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Remarkably, this system is **chaotic** (i.e., it is very sensitive to the initial conditions in long time) and possesses a strange attractor.

This fact, though conjectured since the 1960s, was only proved by Warwick Tucker in 1999, using a computer-assisted proof using interval arithmetic.

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No Dirichlet vertices $\to \gamma_1 = 0$.

The *nonlinear* Schrödinger equation on metric graphs

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When $p = 2$, the solutions of $(\mathcal{P}_p)$ are the eigenfunctions in E_2.

Nodal action ground states

Among all solutions of $(\mathcal{P}_p)$ when $p > 2$, we are particularly interested in nodal action ground states, namely sign-changing solutions which minimize the action functional

$$\mathcal{J}_p(u) := \frac{1}{2}\|u'\|^2_{L^2(\mathcal{G})} + \frac{\lambda}{2}\|u\|^2_{L^2(\mathcal{G})} - \frac{\gamma_2}{p}\|u\|^p_{L^p(\mathcal{G})}$$

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among all nonzero sign-changing solutions of $(\mathcal{P}_p)$.

Question

What is the behavior of nodal action ground states as $p \to 2$?

The quasilinear regime $p \approx 2$ ($p > 2$)

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Let $(p_n)_{n \geq 1} \subseteq]2, +\infty[$ *be a sequence of exponents which converges to* 2

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Let $(p_n)_{n\geq 1} \subseteq]2, +\infty[$ be a sequence of exponents which converges to 2 and $(u_{p_n})_{n\geq 1} \subseteq H^1(\mathcal{G})$ be a sequence of nonzero solutions to the problems $(\mathcal{P}_{p_n})$.

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$$\int_{\mathcal{G}} u_* \ln |u_*| \varphi \, \mathrm{d}x = 0 \qquad \forall \varphi \in E_2.$$

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$$\int_{\mathcal{G}} u_* \ln|u_*| \varphi \, \mathrm{d}x = 0 \qquad \forall \varphi \in E_2.$$

We say that $u_* \in E_2$ is a *solution of the reduced problem* if the above condition holds.

Variational formulation

The functional $\mathcal{J}_* : E_2 \to \mathbb{R}$

$$\mathcal{J}_*(\varphi) := \frac{1}{4} \int_{\mathcal{G}} \varphi^2(x) \big(1 - 2 \ln |\varphi(x)|\big) \, \mathrm{d}x$$

is of class $\mathcal{C}^1$, and the solutions of the reduced problem coincide with its critical points.

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As we saw on part I, a Lyapunov-Schmidt argument, implies **existence and uniqueness results around a nondegenerate critical point** for $(\mathcal{P}_p)$, when $p \approx 2$. *But how to do goals 1 and 2?*

Geometry of $\mathcal{J}_*$

For any $\varphi \in E_2 \setminus \{0\}$, the map

$$]0, +\infty[\to \mathbb{R} : t \mapsto \mathcal{J}_*(t\varphi)$$

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has a unique maximum.

Its value can be computed explicitly and is given by

$$n_*(\varphi) = \exp\left(-\frac{\int_{\mathcal{G}} \varphi^2 \ln|\varphi| \, \mathrm{d}x}{\int_{\mathcal{G}} \varphi^2 \, \mathrm{d}x}\right).$$

The reduced Nehari manifold

The reduced Nehari manifold $\mathcal{N}_*$, defined by

$$\mathcal{N}_* := \left\{ \varphi \in E_2 \setminus \{0\} \;\middle|\; \mathcal{J}_*'(\varphi)[\varphi] = 0 \right\}$$

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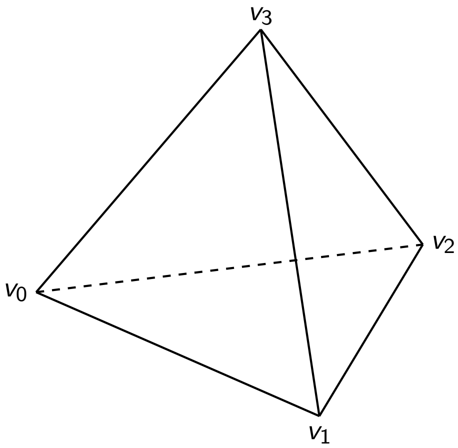
Theorem (Bonheure, Bouchez, Grumiau, Van Schaftingen (2008))

Weak limits of nodal action ground states minimize $\mathcal{J}_*$ over $\mathcal{N}_*$.

The tetrahedron

In the remainder of the talk, we will focus on the following graph $\mathcal{G}_t$.



Second eigenspace of $\mathcal{G}_t$

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where φ_a is such that

$$\varphi_a(x) = \frac{a_i \sin(\sqrt{\gamma_2}(1-x)) + a_j \sin(\sqrt{\gamma_2}x)}{\sin(\sqrt{\gamma_2})},$$

if x belongs to the edge $v_i v_j$.

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What you should remember

Only two things :-)

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   has dimension *three*;

2. a encodes the values of φ_a at the vertices, in the sense that

$$\varphi_a(v_i) = a_i$$

   for all $i \in \{0, 1, 2, 3\}$.

Symmetries of $\mathcal{G}_t$

The group

$$G_t := S_4 \times \{\pm 1\}$$

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acts on E_2 due to the fact that "all vertices of the tetrahedron are the same" and that the functional $\mathcal{J}_*$ is even.

In this way, we obtain an *isometric group action*

$$G_t \times E_2 \to E_2 : (g, \varphi) \mapsto g \cdot \varphi,$$

such that

$$J_*(g \cdot \varphi) = J_*(\varphi)$$

for all $(g, \varphi) \in G_t \times E_2$.

Critical points created by the symmetries

The presence of such a rich symmetry group entails the existence of four distinct families of critical points, due to the *principle of symmetric criticality*.

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then u is a critical point of J.

The families of critical points

Proposition

The following eigenfunctions are critical points of $\mathcal{J}_*$*:*

- $f_0 := \pi_{\mathcal{N}_*}\big(\varphi_{(1,-1,0,0)}\big)$;
- $f_1 := \pi_{\mathcal{N}_*}\big(\varphi_{(1,-1/3,-1/3,-1/3)}\big)$;
- $f_2 := \pi_{\mathcal{N}_*}\big(\varphi_{(1,1,-1,-1)}\big)$;
- $f_3 := \pi_{\mathcal{N}_*}\big(\varphi_{(1,-1,c,-c)}\big)$ *where* $c \in \,]0,1[$ *maximizes the function*

$$[0,1] \to \mathbb{R} : c \mapsto \mathcal{J}_*\big(\pi_{\mathcal{N}_*}\big(\varphi_{(1,-1,c,-c)}\big)\big).$$

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Moreover, for every $g \in G_t$ *and every* $i \in \{0,1,2,3\}$, $g \cdot f_i$ *is a critical point of* $\mathcal{J}_*$.

For instance, f_1 is a critical point of $\mathcal{J}_*$ restricted to the one-dimensional subspace of E_2 taking equal values in v_1, v_2 and v_3.

A natural question

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Does $\mathcal{J}_*$ possess critical points other than the ones of the four aforementioned families?

Answer (De Coster, G., Troestler (2024))

Those are the only critical points as shown by a computer-assisted proof.

What we use the computer for

The main thing we want to prove with the help of the computer is the following proposition.

Proposition

f_0, f_1, f_2 and f_3 are the only nonzero critical points of $\mathcal{J}_*$ up to symmetries, in the sense that

$$\forall \varphi \in E_2 \setminus \{0\}, \left[(\mathcal{J}_*'(\varphi) = 0) \implies (\exists i \in \{0,1,2,3\}, \exists g \in G_t, \varphi = g \cdot f_i) \right].$$

Moreover, f_1, f_2 and f_3 are nondegenerate.

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1. locating small "boxes" containing all critical points of $\mathcal{J}_*$, by root finding methods.
2. proving uniqueness of critical points inside each box using second order information.

Variational characterization of the critical points

Proposition

The action levels of the critical points we found are so that

$$\mathcal{J}_*(f_2) < \mathcal{J}_*(f_0) < \mathcal{J}_*(f_3) < \mathcal{J}_*(f_1).$$

Moreover,

- f_0 *is a* ***strict local minimum*** *of* $\mathcal{J}_*$ *on* $\mathcal{N}_*$*;*
- f_1 *is a strict* ***global maximum*** *of* $\mathcal{J}_*$ *on* $\mathcal{N}_*$*;*
- f_2 *is a strict* ***global minimum*** *of* $\mathcal{J}_*$ *on* $\mathcal{N}_*$*;*
- f_3 *is a* ***saddle point*** *of* $\mathcal{J}_*$ *on* $\mathcal{N}_*$.

Qualitative properties of nodal ground states as $p \to 2$

Theorem

There exists $\delta > 0$ *such that, for every* $p \in]2, 2+\delta]$, *there exists* $\tilde{u}_p$, *a nodal action ground state of* $(\mathcal{P}_p)$, *such that*

$$\tilde{u}_p(v_0) = \tilde{u}_p(v_1) = -\tilde{u}_p(v_2) = -\tilde{u}_p(v_3) > 0.$$

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Moreover, $\tilde{u}_p$ *is unique up to symmetries, in the sense that*

$$\forall u_p \in H^1(\mathcal{G}_{\mathrm{t}}), \Big[u_p \text{ is a nodal action ground state of } (\mathcal{P}_{p,2}) \implies \left(\exists g \in G_t, u_p = g \cdot \tilde{u}_p\right)\Big].$$

Take-home messages

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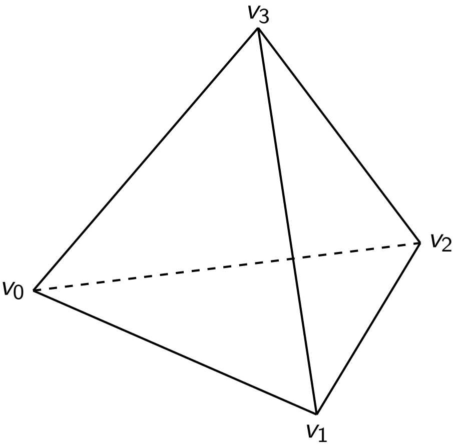
Metric graphs allow to study interesting *one dimensional* problems and are much richer than the usual class of intervals of $\mathbb{R}$. In particular, one may study *highly symmetric examples*.

Computer-assisted methods may allow to prove difficult statements and can be very relevant to study in depth given examples.

Thanks for your attention!



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