

# CONSTRUCTION OF ARTIFICIAL BOUNDARY CONDITIONS FOR DISPERSIVE EQUATIONS

*by*

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TBC for dispersive Eqs.



## THE SCHRÖDINGER EQ. IN $\mathbb{R}$

$$(S) \quad \begin{cases} i\partial_t \psi + \partial_x^2 \psi + V(x, t) \psi = 0, & (x, t) \in \mathbb{R} \times [0; T] \\ \lim_{|x| \rightarrow +\infty} \psi(x, t) = 0, & t \in [0; T] \\ \psi(x, 0) = \psi_0(x), & x \in \mathbb{R} \end{cases}$$

- $\psi(x, t)$ : wave function, complex
- real potential,  $\mathcal{V} = V(x, t) \in C^\infty(\mathbb{R}^d \times \mathbb{R}^+, \mathbb{R})$
- $\psi_0$  compact support in  $\Omega$

- Laplace transform

$$\mathcal{L}_t(u)(x, \omega) = \int_0^\infty u(x, t)e^{-\omega t} dt$$

with the covariable  $\omega = \sigma + i\tau$ ,  $\sigma > 0$

- Fourier transform :

$$\mathcal{F}_t(u)(x, \tau) = \hat{u}(x, \tau) = \frac{1}{2\pi} \int_{\mathbb{R}} u(x, t)e^{-it\tau} dt.$$

- $\mathcal{L}_t(\partial_t u)(x, \omega) = \omega \mathcal{L}_t(u)(x, \omega) - u(x, 0)$
- $\mathcal{F}_t(\partial_t u)(x, \tau) = i\tau \mathcal{F}_t(u)(x, \tau)$

## PSEUDODIFFERENTIAL OPERATORS IN 1D

- A pseudodifferential operator  $P(x, t, \partial_t)$  is described by its total symbol  $p(x, t, \tau)$  in the Fourier space ( $\tau$  is the covariable of  $t$ )

$$P(x, t, \partial_t) u(x, t) = \mathcal{F}_t^{-1} (p(x, t, \tau) \hat{u}(x, \tau)) = \int_{\mathbb{R}} p(x, t, \tau) \hat{u}(x, \tau) e^{it\tau} d\tau$$

Notations:  $P = Op(p)$  ,  $p(x, t, \tau) = \sigma(P(x, t, \partial_t))$

- Let  $\alpha \in \mathbb{R}$  and the open set  $\Xi \subset \mathbb{R}$ . **Symbol class:**  $S^\alpha(\Xi \times \Xi)$  vector space of functions  $a(x, t, \tau) \in C^\infty(\Xi \times \Xi \times \mathbb{R})$  s.t.  $\forall K \subseteq \Xi \times \Xi$  and  $\beta, \delta, \gamma$ ,  $\exists C_{\beta, \delta, \gamma}(K)$  s.t.

$$|\partial_\tau^\beta \partial_t^\delta \partial_x^\gamma a(x, t, \tau)| \leq C_{\beta, \delta, \gamma}(K) (1 + |\tau|)^{\alpha - \beta},$$

$\forall (x, t) \in K$  and  $\tau \in \mathbb{R}$ .

- The **order** of  $P$  is the homogeneity order of its symbol w.r.t  $\tau$ .

$P(x, t, \partial_t)$  homogeneous of order  $m$  if and only if for  $\mu > 0$ ,  
 $p(x, t, \mu\tau) = \mu^m p(x, t, \tau)$ .



## ASYMPTOTIC EXPANSION IN HOMOGENEOUS SYMBOLS

$P$  is said to be of order  $M$ ,  $M \in \mathbb{Z}/2$ , if:

$$p(x, t, \tau) \sim \sum_{j=0}^{+\infty} p_{M-j/2}(x, t, \tau), \quad \begin{array}{l} p_M = \text{principal symbol of } P \\ P \in OPS^m \text{ and } p \in S^m \end{array}$$

where  $p_{M-j/2}$  is homogeneous of order  $2M - j$  and  $P_{M-j/2} : H^s \rightarrow H^{s+M-j/2}$ .

Meaning of  $\sim$  :  $\forall \tilde{m} \in \mathbb{N}$ ,  $p - \sum_{j=0}^{\tilde{m}} p_{M-j/2} \in S^{M-(\tilde{m}+1)/2}$ .

## Symbolic calculus

## COMPOSITION RULE

$$\sigma(AB) = \sum_{\alpha=0}^{+\infty} \frac{(-i)^\alpha}{\alpha!} \partial_\tau^\alpha \sigma(A) \partial_t^\alpha \sigma(B)$$

If  $A \in OPS^m$  and  $B \in OPS^n$ , then  $AB \in OPS^{m+n}$ .

## EXAMPLES

THE FRACTIONAL OPERATORS  $\partial_t^{1/2}$  AND  $I_t^{\alpha/2}$

$$\partial_t^{1/2} f(t) = \frac{1}{\sqrt{\pi}} \partial_t \int_0^t \frac{f(s)}{\sqrt{t-s}} ds$$

$$I_t^{\alpha/2} f(t) = \frac{1}{\Gamma(\alpha/2)} \int_0^t (t-s)^{\alpha/2-1} f(s) ds$$

Nonlocal w.r.t time  
convolution operator

Operator	$\partial_t$	$\partial_t^{1/2}$	$I_t^{1/2}$	$I_t$
	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$
Symbol	$i\tau$	$e^{-i\pi/4} \sqrt{-\tau}$	$\frac{e^{i\pi/4}}{\sqrt{-\tau}}$	$\frac{1}{i\tau}$
Class	$OPS^1$	$OPS^{1/2}$	$OPS^{-1/2}$	$OPS^{-1}$

## PROPERTIES W.R.T DERIVATIVES

- Let  $A \in OPS^m$ :  $\partial_\tau A \in OPS^{m-1}$ ,  $\partial_{t,x} A \in OPS^m$
- $\partial_x P = Op(\partial_x p) + P\partial_x$ ,  $\sigma(\partial_x P) = \partial_x p + \sigma(P\partial_x)$

FRACTIONAL OPERATOR  $\partial_t^{1/2}$  ET  $I_t^{\alpha/2}$ 

$$\partial_t^{1/2} f(t) = \frac{1}{\sqrt{\pi}} \partial_t \int_0^t \frac{f(s)}{\sqrt{t-s}} ds, \quad \sigma(\partial_t^{1/2}) = e^{-i\pi/4} \sqrt{-\tau} \in S^{1/2}$$

$$I_t^{\alpha/2} f(t) = \frac{1}{\Gamma(\alpha/2)} \int_0^t (t-s)^{\alpha/2-1} f(s) ds, \quad \sigma(I_t^{\alpha/2}) = \left(\frac{i}{\tau}\right)^{\alpha/2} \in S^{-\alpha/2}$$

- CASE  $\mathcal{V} = 0$

TBC:  $\partial_{\mathbf{n}}\psi + e^{-i\pi/4}\partial_t^{1/2}\psi = 0, \quad \text{on } \Sigma_T.$

- CASE CONSTANT  $\mathcal{V} = V$

TBC:  $\partial_{\mathbf{n}}\psi + e^{-i\pi/4}e^{itV}\partial_t^{1/2}(e^{-itV}\psi) = 0, \quad \text{on } \Sigma_T.$

- CASE  $\mathcal{V} = 0$

TBC:  $\partial_{\mathbf{n}}\psi + e^{-i\pi/4}\partial_t^{1/2}\psi = 0, \quad \text{on } \Sigma_T.$

$$\partial_{\mathbf{n}}\psi - iOp(\sqrt{-\tau})\psi = 0, \quad \text{on } \Sigma_T.$$

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$$\partial_{\mathbf{n}}\psi - iOp(\sqrt{-\tau + V})(\psi) = 0, \quad \text{on } \Sigma_T.$$

### LEMMA

If  $a$  is a symbol belonging to  $S^m$  independent of  $t$ , and  $V = V(x)$ , then

$$Op(a(\tau - V(x)))\psi = e^{itV(x)}Op(a(\tau))(e^{-itV(x)}\psi)$$

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- CASE  $\mathcal{V} = V(t)$  : GAUGE CHANGE

 Antoine, Besse et Descombes, 2006

$$\partial_{\mathbf{n}}\psi - ie^{i\mathcal{V}(t)}Op(\sqrt{-\tau})(e^{-i\mathcal{V}(t)}\psi) = 0, \quad \text{on } \Sigma_T.$$

If  $\mathcal{V} = V(x, t) = x$ , by Fourier transform, the Eq.  $i\partial_t u + \partial_x^2 u + xu = 0$  becomes the Airy Eq.

$$\partial_x^2 \hat{u} + (-\tau + x)\hat{u} = 0$$

So  $\hat{u} = \text{Ai}\left((x - \tau)e^{-i\pi/3}\right)$  and we have the **TBC**

$$\partial_n u + e^{2i\pi/3} \text{Op}\left(\frac{\text{Ai}'\left((x - \tau)e^{-i\pi/3}\right)}{\text{Ai}\left((x - \tau)e^{-i\pi/3}\right)}\right)(u) = 0.$$



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$$\partial_{\mathbf{n}} u + e^{2i\pi/3} \text{Op}\left(\frac{\text{Ai}'\left((x - \tau)e^{-i\pi/3}\right)}{\text{Ai}\left((x - \tau)e^{-i\pi/3}\right)}\right)(u) = 0.$$

In a first approximation

$$\frac{\text{Ai}'\left((x - \tau)e^{-i\pi/3}\right)}{\text{Ai}\left((x - \tau)e^{-i\pi/3}\right)} \approx -e^{-i\pi/6} \sqrt[3]{-\tau + x}$$

and one has the **ABC**

$$\partial_{\mathbf{n}} u + i\text{Op}\left(-\sqrt[3]{-\tau + x}\right)(u) = 0, \quad (x, t) \in \Sigma_T$$

which leads to

$$\partial_{\mathbf{n}} u + e^{itx} e^{-i\pi/4} \partial_t^{1/2} \left(e^{-itx} u\right) = 0, \quad (x, t) \in \Sigma_T$$


**REMARK** there exists a change of unknown s.t. if  $v$  is solution to  $i\partial_t v + \partial_x^2 v = 0$ , then

$$u(x, t) = e^{-i(-\alpha t x + \frac{t^3}{3} |\alpha|^2)} v(x - t^2 \alpha, t)$$

is solution to

$$i\partial_t u + \partial_x^2 u + \alpha x u = 0.$$

Therefore, one can work on the free Schrödinger equation.

Changes of unknown are also available for the cases  $V(x) = \pm x^2$  by *lens transform* ( R. Carles (05)).

## PARTIAL CONCLUSION

- We have factorized the operator

$$i\partial_t + \partial_x^2 + V = \left(\partial_x + i\sqrt{i\partial_t + V}\right)\left(\partial_x - i\sqrt{i\partial_t + V}\right)$$

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- TBCs and ABCs are written through a DtN op.

$$\partial_{\mathbf{n}}u + iOp\left(-\sqrt{-\tau}\right)(u) = 0 \quad \text{on } \Sigma_T$$

or

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- if  $\mathcal{V} = V(t)$ , **the change of unknowns**  $v(x, t) = e^{-i\mathcal{V}(t)}u(x, t)$  with  $\mathcal{V}(t) = \int_0^t V(s)ds$  reduces the Schrödinger Eq. with potential to a free Schrödinger Eq. and the TBC is

$$\partial_{\mathbf{n}}u(x, t) + e^{-i\frac{\pi}{4}} e^{i\mathcal{V}(t)} \partial_t^{1/2} \left( e^{-i\mathcal{V}(t)}u \right) (x, t) = 0 \quad \text{on } \Sigma_T$$

1D SCHRÖDINGER EQ.  $\mathcal{V} = V(x, t)$ 

$$\begin{aligned}
 \text{(Syst1)} \quad & i\partial_t \psi + \partial_x^2 \psi + \mathcal{V}\psi = 0, \quad (x, t) \in \mathbb{R}_x \times [0; T], \\
 & \lim_{|x| \rightarrow \infty} \psi(x, t) = 0, \\
 & \psi(x, 0) = \psi_0(x), \quad x \in \mathbb{R}_x.
 \end{aligned}$$

In the general case  $V(x, t)$ , we can not expect to derive a TBC.

Use the symbolic calculus to determine ABCs.

High frequency solution: Engquist-Majda method

Admissible potentials class: repulsive potentials

## REPULSIVE POTENTIAL

$V$  smooth and  $x\partial_x V(x, t) > 0$  for  $x \in \bar{\Omega}$ ,  $t > 0$ .

Ex :  $V(x, t) = x^2$

## Two strategies

## GAUGE CHANGE (STRATEGY 1)

- Change of unknown (this solves the case  $\mathcal{V} = V(t)$ ):  $v = e^{-i\mathcal{V}}u$  with  $\mathcal{V}(x, t) = \int_0^t V(x, s) ds$  where  $f = 2i\partial_x \mathcal{V}$  et  $g = i\partial_x^2 \mathcal{V} - (\partial_x \mathcal{V})^2$ .
- We work with the equation for  $v$  :

$$i\partial_t v + \partial_x^2 v + f \partial_x v + g v = 0$$

## DIRECT METHOD (STRATEGY 2)

- One works directly on the original equation

$$i\partial_t u + \partial_x^2 u + V u = 0$$

$\Rightarrow$  Boundary conditions for  $i\partial_t w + \partial_x^2 w + A \partial_x w + B w = 0$ , with

- $A = 0$  and  $B = V(x, t)$  if  $w = u$ ,
- $A = f(x, t)$  and  $B = g(x, t)$  if  $w = ve^{-i\mathcal{V}}u$ .

General Schrödinger operator:  $L = i\partial_t + \partial_x^2 + A \partial_x + B$

FACTORIZATION OF THE OPERATOR  $L$  (NIRENBERG)

$$L = i\partial_t + \partial_x^2 + A\partial_x + B = (\partial_x + i\Lambda^-)(\partial_x + i\Lambda^+) + R$$

$\Lambda^\pm \in \text{OPS}^{1/2}$  and  $R \in \text{OPS}^{-\infty}$

$\Lambda^+$  has an asymptotic expansion in homogeneous symbols:

$$\sigma(\Lambda^+) = \lambda^+ \sim \sum_{j=0}^{+\infty} \lambda_{1/2-j/2}^+ = \lambda_{1/2}^+ + \lambda_0^+ + \lambda_{-1/2}^+ + \lambda_{-1}^+ + \dots$$

with  $\lambda_{1/2-j/2}^+$  homogeneous of order  $1/2 - j/2$ .

ARTIFICIAL CONDITION :  $\partial_{\mathbf{n}}w + i\Lambda^+w = 0$

$$\partial_{\mathbf{n}}w + i \sum_{j=0}^{+\infty} \text{Op} \left( \lambda_{1/2-j/2}^+ \right) w = 0, \quad \text{on } \Sigma_T$$

APPROXIMATED CONDITION OF ORDER  $M$ :

$$\partial_{\mathbf{n}}w_M + i \sum_{j=0}^{M-1} \text{Op} \left( \lambda_{1/2-j/2}^+ \right) w_M = 0, \quad \text{on } \Sigma_T$$



## IDENTIFICATION OF THE INVOLVED TERMS

Thanks to  $\partial_x \Lambda^+ = Op(\partial_x \Lambda^+) + \Lambda^+ \partial_x$ , we have

- $L = \partial_x^2 + A\partial_x + i\partial_t + B$
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- $L = \partial_x^2 + A\partial_x + i\partial_t + B$
- $(\partial_x + i\Lambda^-)(\partial_x + i\Lambda^+) = \partial_x^2 + i(\Lambda^+ + \Lambda^-)\partial_x + iOp(\partial_x \Lambda^+) - \Lambda^- \Lambda^+$
- Identification of the coefficients (up to  $R$ )

$$\begin{aligned} i(\Lambda^- + \Lambda^+) &= A \\ iOp(\partial_x \Lambda^+) - \Lambda^- \Lambda^+ &= i\partial_t + B \end{aligned}$$

- Symbolic system

$$\begin{aligned} i(\lambda^- + \lambda^+) &= a \\ i\partial_x \lambda^+ - \sum_{\alpha=0}^{\infty} \frac{(-i)^\alpha}{\alpha!} \partial_\tau^\alpha \partial_t^\alpha \lambda^+ &= -\tau + b \end{aligned}$$

- Since  $\lambda^\pm \sim \sum_{j=0}^{+\infty} \lambda_{1/2-j/2}^\pm$ , we compute  $\lambda_{1/2-j/2}^\pm$  by identification of the terms of same order in the system.

The principal symbol with negative real part characterizes the **outgoing wave** of  $u$

- **STRATEGY 1:** Case  $A = f$  and  $B = g$ . We choose

$$\lambda_{1/2}^+ = -\sqrt{-\tau} \quad (S1)$$

- **STRATEGY 2:** Case  $A = 0$  and  $B = V$ . We choose

$$\lambda_{1/2}^+ = -\sqrt{-\tau + V} \quad (S2).$$

Remark: for the second strategy, we could also have chosen  $\lambda_{1/2}^+ = -\sqrt{-\tau}$ . This choice would lead to a less accurate ABC since it would give some symbols which are approx. of  $-\sqrt{-\tau + V}$  when  $|\tau| \rightarrow +\infty$ .

STRATEGY 1: GAUGE CHANGE  $v = e^{-i\mathcal{V}}u$ 

- 

$$\lambda_{1/2}^+ = -\sqrt{-\tau}, \quad \lambda_0^+ = \partial_x \mathcal{V}, \quad \lambda_{-1/2}^+ = 0, \quad \lambda_{-1}^+ = \frac{i\partial_x V}{4\tau}$$

- Interpretation of symbols

$$Op(-\sqrt{-\tau}) = e^{-3i\pi/4} \partial_t^{1/2}$$

$$Op\left(\frac{i\partial_x V}{4\tau}\right) = \frac{\partial_n V}{4} I_t \quad \text{or} \quad \text{sg}(\partial_n V) \frac{\sqrt{|\partial_n V|}}{2} \frac{\sqrt{|\partial_n V|}}{2} I_t$$

STRATEGY 2: DIRECT METHOD  $A = 0, B = V$ 

- 

$$\lambda_{1/2}^+ = -\sqrt{-\tau + V}, \quad \lambda_0^+ = 0, \quad \lambda_{-1/2}^+ = 0, \quad \lambda_{-1}^+ = -\frac{i}{4} \frac{\partial_x V}{-\tau + V}$$

- Interpretation of symbols

$$\begin{aligned} Op\left(-\sqrt{-\tau + V}\right) &= \sqrt{i\partial_t + V} \bmod OPS^{-3/2} \\ Op\left(\frac{\partial_x V}{-\tau + V}\right) &= \partial_n V (i\partial_t + V)^{-1} \bmod OPS^{-5/2} \end{aligned}$$

Comparison for  $V(x, t) = x$

$$\lambda^+ = e^{2i\pi/3} \frac{\text{Ai}'\left((x - \tau)e^{-i\pi/3}\right)}{\text{Ai}\left((x - \tau)e^{-i\pi/3}\right)}.$$

with

$$\lambda = i\lambda_{1/2}^+ + i\lambda_{-1}^+ = -i\sqrt{-\tau + x} + \frac{1}{4} \frac{1}{-\tau + x}$$

Abramowitz-Stegun :  $\lambda^{+, (2)}$  is actually the asymptotic expansion of  $\lambda^+$  for large enough  $\tau$ .



- STRATEGY 1: ABC is  $\partial_{\mathbf{n}}v + i\Lambda^+v = 0$  on  $\Sigma_T$ . But  $v(x, t) = e^{-i\mathcal{V}(x, t)}u(x, t)$ . Therefore, for  $u$ , retaining the  $M$  first symbols, we have

$$\partial_{\mathbf{n}}u - i(\partial_x \mathcal{V})u + ie^{i\mathcal{V}} \sum_{j=0}^{M-1} Op\left(\lambda_{1/2-j/2}^{+, (1)}\right) \left(e^{-i\mathcal{V}}u\right) = 0, \quad \text{on } \Sigma_T,$$

- STRATEGY 2: ABC is  $\partial_{\mathbf{n}}u + i\Lambda^+u = 0$

$$\partial_{\mathbf{n}}u + i \sum_{j=0}^{M-1} Op\left(\lambda_{1/2-j/2}^{+, (2)}\right) u = 0 \quad \text{on } \Sigma_T.$$

- **STRATEGY 1:** For reason of symmetry and to get adequate estimates, the ABC of 4<sup>th</sup> order **ABC<sub>1</sub><sup>4</sup>** is

$$\partial_{\mathbf{n}}u + e^{-i\pi/4} e^{i\mathcal{V}(x,t)} \partial_t^{1/2} \left( e^{-i\mathcal{V}(x,t)} u \right) \quad (\text{ABC}_1^2)$$

$$+ i \operatorname{sg}(\partial_{\mathbf{n}}V) \frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2} e^{i\mathcal{V}(x,t)} I_t \left( \frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2} e^{-i\mathcal{V}(x,t)} u \right) = 0$$

- **STRATEGY 2:** The ABC of 4<sup>th</sup> order **ABC<sub>2</sub><sup>4</sup>** is

$$\partial_{\mathbf{n}}u + i\sqrt{i\partial_t + V} u \quad (\text{ABC}_2^2) + \frac{i}{4} \partial_{\mathbf{n}}V (i\partial_t + V)^{-1} u = 0$$

**PROPOSITION** Let  $u_0 \in L^2(\Omega)$  s.t.  $\text{Supp}(u_0) \subset \Omega$ . Let  $V \in C^\infty(\mathbb{R} \times \mathbb{R}^+, \mathbb{R})$  and  $u$  a solution of

$$\begin{cases} i\partial_t u + \partial_x^2 u + V u = 0, & \text{in } \Omega_T, \\ \partial_n u + \Lambda_1^M u = 0, & \text{on } \Sigma_T, \\ u(x, 0) = u_0(x), & \forall x \in \Omega, \end{cases}$$

where

$$\Lambda_1^2(x, t, \partial_t) u = e^{-i\pi/4} e^{i\mathcal{V}(x,t)} \partial_t^{1/2} \left( e^{-i\mathcal{V}(x,t)} u \right)$$

and

$$\Lambda_1^4(x, t, \partial_t) u = \Lambda_1^2(x, t, \partial_t) u + i \text{sg}(\partial_n V) \frac{\sqrt{|\partial_n V|}}{2} e^{i\mathcal{V}(x,t)} I_t \left( \frac{\sqrt{|\partial_n V|}}{2} e^{-i\mathcal{V}(x,t)} u \right)$$

Then,  $u$  fulfils the following energy bound

$$\forall t > 0, \quad \|u(t)\|_{L^2(\Omega)} \leq \|u_0\|_{L^2(\Omega)},$$

for  $M = 2$  and for  $M = 4$  if  $\text{sg}(\partial_n V)$  is constant on  $\Sigma_T$ , which implies the uniqueness of the solution.

In the case of strategy 2, we have

$$\partial_{\mathbf{n}} u + \Lambda_2^M u = 0, \quad \text{on } \Sigma_T,$$

with

$$\Lambda_2^2(x, t, \partial_t) u = Op\left(-i\sqrt{-\tau + V}\right) u$$

and

$$\Lambda_2^4(x, t, \partial_t) u = \Lambda_2^2(x, t, \partial_t) u + \frac{1}{4} Op\left(\frac{\partial_x V}{-\tau + V}\right) u$$

If  $V(x, t) = V(x)$ ,  $ABC_2^M$  and  $ABC_1^M$  are strictly equivalent.

$$\begin{cases} i\partial_t u + \partial_x^2 u + V u = 0, & \text{in } \Omega_T \\ u(\cdot, 0) = u_0, & \text{in } \Omega \end{cases}$$

with ABC on  $\Sigma_T$ , for  $M = 2$  or  $4$

### STRATEGY 1

$$ABC_1^2 \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} (e^{-i\mathcal{V}} u) = 0,$$

$$ABC_1^4 \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} (e^{-i\mathcal{V}} u) \\ + i \operatorname{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{i\mathcal{V}(x,t)} I_t \left( \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{-i\mathcal{V}(x,t)} u \right) = 0.$$

or

### STRATEGY 2

$$ABC_2^2 \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V} u = 0,$$

$$ABC_2^4 \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V} u \\ + \operatorname{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} (i\partial_t + V)^{-1} \left( \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} u \right) = 0.$$

Let  $\Delta t = T/N$  be the time step and let us set  $t_n = n\Delta t$  and  $u^n$  stands for an approximation of  $u(t_n)$ .

- **Time approximation** Semi-discrete Crank-Nicolson *symmetrical* scheme

$$i \frac{u^{n+1} - u^n}{\Delta t} + \partial_x^2 \left( \frac{u^{n+1} + u^n}{2} \right) + \frac{V^{n+1} + V^n}{2} \frac{u^{n+1} + u^n}{2} = 0,$$

for  $n = 0, \dots, N - 1$ .

Implementation

$$2i \frac{v^{n+1}}{\Delta t} + \partial_x^2 v^{n+1} + W^{n+1} v^{n+1} = 2i \frac{u^n}{\Delta t}$$

with  $v^{n+1} = (u^{n+1} + u^n)/2 = u^{n+1/2}$ ,  $W^{n+1} = (V^{n+1} + V^n)/2 = V^{n+1/2}$ .

The symmetry is fundamental to guarantee the stability of the numerical scheme.

- **Space approximation** Finite Element Method
  - $ABC_1^M$ : discrete convolutions
  - $ABC_2^M$ : rational approximation of the square root (Padé)

## STRATEGY 1

$$\begin{cases} i\partial_t u + \partial_x^2 u + V u = 0, & \text{in } \Omega_T \\ \partial_{\mathbf{n}} u + \Lambda_1^M u = 0, & \text{on } \Sigma_T, \text{ for } M = 2 \text{ ou } 4 \\ u(\cdot, 0) = u_0, & \text{in } \Omega \end{cases}$$

with

$$ABC_1^2 \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} (e^{-i\mathcal{V}} u) = 0,$$

$$ABC_1^4 \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} (e^{-i\mathcal{V}} u) \\ + i \operatorname{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{i\mathcal{V}(x,t)} I_t \left( \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} e^{-i\mathcal{V}(x,t)} u \right) = 0.$$

## NUMERICAL SCHEME FOR $ABC_1^M$ : DISCRETE CONVOLUTIONS

Approximations of  $\partial_t^{1/2}$ ,  $I_t^{1/2}$  and  $I_t$  in agreement with the Crank-Nicolson scheme  
 $\Rightarrow$  trapezoidal formula [Schmidt-Yevick (97), Antoine-Besse (03)]

$$\begin{aligned} \partial_t^{1/2} f(t^n) &\approx \sqrt{\frac{2}{\Delta t}} \sum_{k=0}^n \beta_{n-k} f^k \\ I_t^{1/2} f(t^n) &\approx \sqrt{\frac{\Delta t}{2}} \sum_{k=0}^n \alpha_{n-k} f^k \\ I_t f(t^n) &\approx \frac{\Delta t}{2} \sum_{k=0}^n \gamma_{n-k} f^k \end{aligned} \quad \left\{ \begin{array}{l} (\alpha_0, \alpha_1, \alpha_2, \dots) = (1, 1, \frac{1}{2}, \frac{1}{2}, \frac{3}{8}, \frac{3}{8}, \dots) \\ \beta_k = (-1)^k \alpha_k, \quad \forall k \geq 0, \\ (\gamma_0, \gamma_1, \gamma_2, \dots) = (1, 2, 2, \dots) \end{array} \right.$$

### PROPOSITION

Let  $u^n$  be the solution to the problem with the boundary conditions  $ABC_1^M$  discretized with discrete convolutions. For  $M = 2$ , we have

$$\forall n \in \{0, \dots, N\}, \quad \|u^n\|_{L^2(\Omega)} \leq \|u^0\|_{L^2(\Omega)},$$

and if  $\partial_n W^k$  has a constant sign, also true for  $M = 4$ .

$\Rightarrow$  The unconditional stability of the scheme is preserved.



## STRATEGY 2

$$\begin{cases} i\partial_t u + \partial_x^2 u + V u = 0, & \text{in } \Omega_T \\ \partial_{\mathbf{n}} u + \Lambda_2^M u = 0, & \text{on } \Sigma_T, \text{ for } M = 2 \text{ or } 4 \\ u(\cdot, 0) = u_0, & \text{in } \Omega \end{cases}$$

with

$$ABC_2^2 \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V} u = 0,$$

$$ABC_2^4 \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V} u \\ + \operatorname{sg}(\partial_{\mathbf{n}} V) \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} (i\partial_t + V)^{-1} \left( \frac{\sqrt{|\partial_{\mathbf{n}} V|}}{2} u \right) = 0.$$

## NUMERICAL SCHEME FOR $ABC_2^M$

The square root is approximated by Padé approximants of order  $m$ :

$$\sqrt{z} \approx R_m(z) = \sum_{k=0}^m a_k^m - \sum_{k=1}^m \frac{a_k^m d_k^m}{z + d_k^m},$$

$$\text{with } a_0^m = 0, \quad a_k^m = \frac{1}{m \cos^2\left(\frac{(2k+1)\pi}{4m}\right)}, \quad d_k^m = \tan^2\left(\frac{(2k+1)\pi}{4m}\right).$$

For the conditions  $ABC_2^M$  :

$$\begin{aligned} \sqrt{i\partial_t + V} &\rightsquigarrow R_m(i\partial_t + V) \\ \Rightarrow \sqrt{i\partial_t + V} &\approx \left( \sum_{k=0}^m a_k^m \right) u - \sum_{k=1}^m a_k^m d_k^m \underbrace{(i\partial_t + V + d_k^m)^{-1} u}_{\varphi_k} \end{aligned}$$

*Lindmann's trick (85) : introduction of auxiliary functions*

$$i\partial_t \varphi_k + (V + d_k^m) \varphi_k = u, \quad \text{pour } 1 \leq k \leq m, \quad \text{in } x = x_{l,r},$$

with  $\varphi_k(x, 0) = 0$ .

The ABC becomes for the semi-discrete scheme

$$\begin{cases} \partial_{\mathbf{n}} v^{n+1} - i \sum_{k=0}^m a_k^m v^{n+1} + i \sum_{k=1}^m a_k^m d_k^m \varphi_k^{n+1/2} = 0, \\ i \frac{\varphi_k^{n+1} - \varphi_k^n}{\Delta t} + (W^{n+1} + d_k^m) \varphi_k^{n+1/2} = v^{n+1}, \\ \varphi_k^0 = 0. \end{cases}$$

For  $ABC_2^4$

$$\partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V}u + \text{sg}(\partial_{\mathbf{n}}V) \frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2} (i\partial_t + V)^{-1} \left( \frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2} u \right) = 0,$$

we introduce an auxiliary function  $\psi$  s.t.

$$(i\partial_t + V)\psi = \frac{\sqrt{|\partial_{\mathbf{n}}V|}}{2} u.$$

No stability results

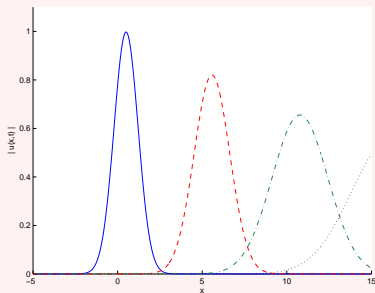
## Exact solutions profile

Gaussian initial data  $u_0(x) = e^{-x^2 + ik_0 x}$ ,  $k_0 = 10$ .

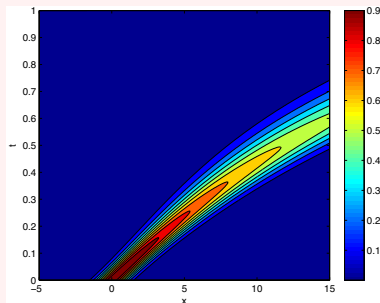
$$V(x) = x^2$$

$$\Omega_T = [-5; 15] \times [0, 1]$$

repulsive potential

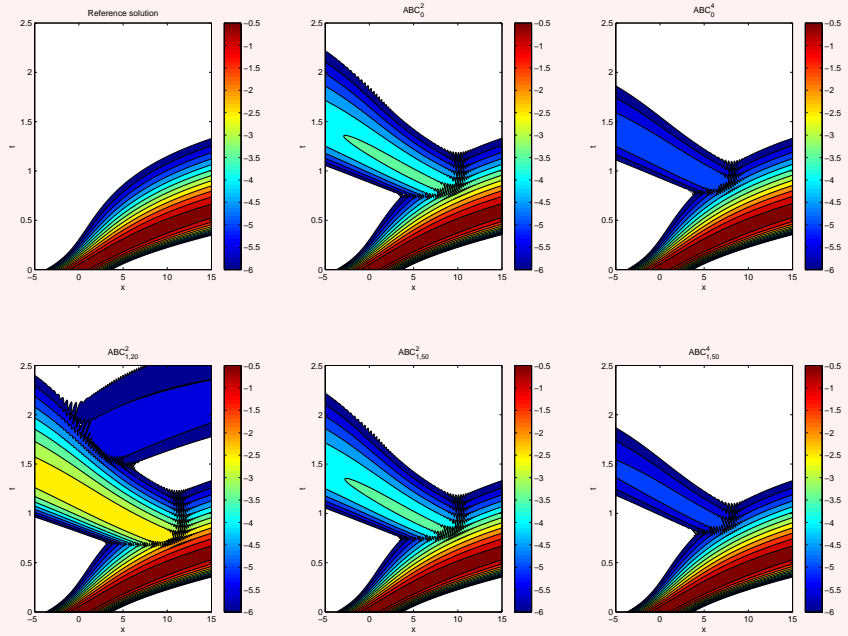


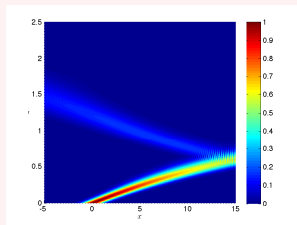
Evolution for different times



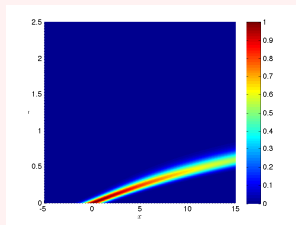
Plot of  $|u|$  in plane  $(x, t)$

# APPLICATIONS $\mathcal{V} = x^2$

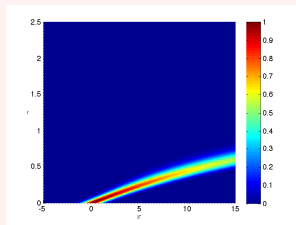




ABC<sup>0</sup>



ABC<sup>2</sup>



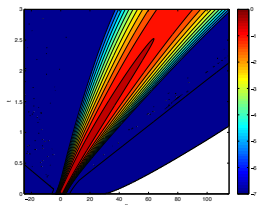
ABC<sup>4</sup>

Application to a potential  $V(x, t) : \mathcal{V} = x(2 + \cos(2t))$

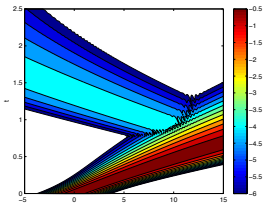
Computational domain  $\Omega_T = [-5; 15] \times [0; 2.5]$

$\Delta x = 2.5 \cdot 10^{-3}$ ,  $\Delta t = 10^{-3}$ , 50 Padé functions,

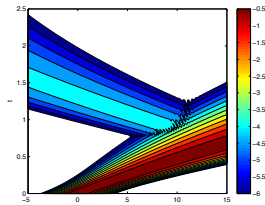
**Logarithmic scale**



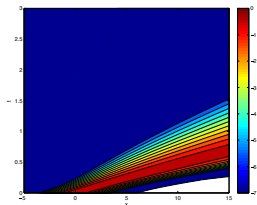
Reference solution computed on a wide domain  $[-25; 115]$



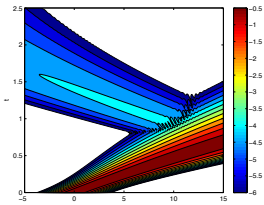
$ABC_1^2 \quad 10^{-4}$



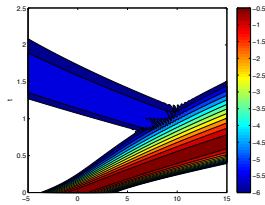
$ABC_1^4 \quad 10^{-4}$



Truncated reference solution



$ABC_2^2 \quad 10^{-4}$



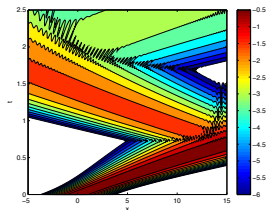
$ABC_2^4 \quad 10^{-5.5}$

Application to a potential  $V(x, t) : \mathcal{V} = x(2 + \cos(2t))$

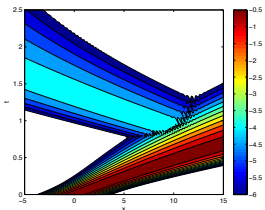
Computational domain  $\Omega_T = [-5; 15] \times [0; 2.5]$

$\Delta x = 2.5 \cdot 10^{-3}$ ,  $\Delta t = 10^{-3}$ , 50 Padé functions,

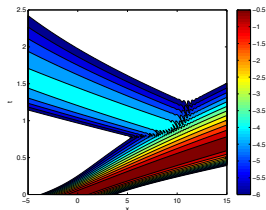
**Logarithmic scale**



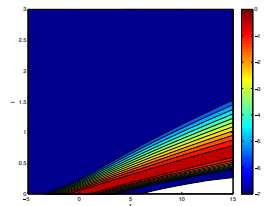
TBC  $10^{-1.5}$



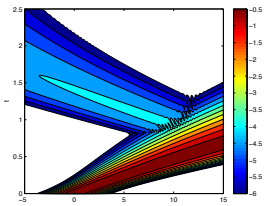
ABC<sub>1</sub><sup>2</sup>  $10^{-4}$



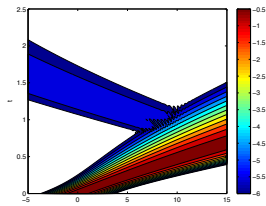
ABC<sub>1</sub><sup>4</sup>  $10^{-4}$



Truncated reference solution



ABC<sub>2</sub><sup>2</sup>  $10^{-4}$



ABC<sub>2</sub><sup>4</sup>  $10^{-5.5}$



- $\mathcal{V} = 0$  WITHOUT POTENTIAL

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} \partial_t^{1/2} u = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = V$  CONSTANT

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} e^{itV} \partial_t^{1/2} \left( e^{-itV} u \right) = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = V(t)$ : GAUGE CHANGE

Setting  $v(x, t) = u(x, t) e^{-i\mathcal{V}(t)}$  with  $\mathcal{V}(t) = \int_0^t V(s) ds$ ,

then  $v$  is solution of the free-potential equation.

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}(t)} \partial_t^{1/2} \left( e^{-i\mathcal{V}(t)} u \right) = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = 0$  WITHOUT POTENTIAL

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} \partial_t^{1/2} u = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = V$  CONSTANT

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} e^{itV} \partial_t^{1/2} \left( e^{-itV} u \right) = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = V(t)$ : GAUGE CHANGE

Setting  $v(x, t) = u(x, t) e^{-i\mathcal{V}(t)}$  with  $\mathcal{V}(t) = \int_0^t V(s) ds$ ,

then  $v$  is solution of the free-potential equation.

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}(t)} \partial_t^{1/2} \left( e^{-i\mathcal{V}(t)} u \right) = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = 0$  WITHOUT POTENTIAL

$$\partial_{\mathbf{n}} u - i \text{Op}(\sqrt{-\tau}) u = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = V$  CONSTANT

$$\partial_{\mathbf{n}} u - i e^{itV} \text{Op}(\sqrt{-\tau}) \left( e^{-itV} u \right) = 0 \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = V(t)$ : GAUGE CHANGE

Setting  $v(x, t) = u(x, t) e^{-i\mathcal{V}(t)}$  with  $\mathcal{V}(t) = \int_0^t V(s) ds$ ,

then  $v$  is solution of the free-potential equation.

$$\partial_{\mathbf{n}} u - i e^{i\mathcal{V}(t)} \text{Op}(\sqrt{-\tau}) \left( e^{-i\mathcal{V}(t)} u \right) = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = 0$  WITHOUT POTENTIAL

$$\partial_{\mathbf{n}} u - i \operatorname{Op}(\sqrt{-\tau}) u = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = V$  CONSTANT

$$\partial_{\mathbf{n}} u - i e^{itV} \operatorname{Op}(\sqrt{-\tau}) \left( e^{-itV} u \right) = 0 \quad \text{on } \Sigma_T.$$

$$\partial_{\mathbf{n}} u - i \operatorname{Op}(\sqrt{-\tau + V}) (u) = 0, \quad \text{on } \Sigma_T.$$

- $\mathcal{V} = V(t)$ : GAUGE CHANGE

Setting  $v(x, t) = u(x, t) e^{-i\mathcal{V}(t)}$  with  $\mathcal{V}(t) = \int_0^t V(s) ds$ ,

then  $v$  is solution of the free-potential equation.

$$\partial_{\mathbf{n}} u - i e^{i\mathcal{V}(t)} \operatorname{Op}(\sqrt{-\tau}) \left( e^{-i\mathcal{V}(t)} u \right) = 0, \quad \text{on } \Sigma_T.$$

## 1) GAUGE CHANGE

- $v(x, t) = e^{-i\mathcal{V}(x, t)} u(x, t)$ , with  $\mathcal{V}(x, t) = \int_0^t V(x, s) ds$ .

- No longer exact

- Involves operators  $e^{i\mathcal{V}(x, t)} Op(\sqrt{-\tau}) (e^{-i\mathcal{V}(x, t)} u)$

$$ABC_1^4 : \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} (e^{-i\mathcal{V}} u) + i \frac{\partial_{\mathbf{n}} V}{4} e^{i\mathcal{V}} I_t (e^{-i\mathcal{V}} u) = 0$$

## 2) DIRECT METHOD

- No gauge change

- Involves operators  $Op(\sqrt{-\tau + V(x, t)})(u)$

$$\widetilde{ABC}_2^4 : \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V} u + \frac{1}{4} \partial_{\mathbf{n}} V (i\partial_t + V)^{-1} u = 0$$

- Strategies equivalent for  $V = V(x)$ , non equivalent for  $V = V(x, t)$

- In both cases, **approximate** boundary conditions, of different orders  $M$ .

NONLINEARITY  $f(u) = g(|u|^2)$

- Cubic  $f(u) = q|u|^2$  / quintic  $f(u) = q|u|^4$
- $f(u) = n_2|u|^2 + n_4|u|^4$ ,  $f(u) = \frac{|u|^2}{1+\sigma|u|^2}$
- Mixed:  $\mathcal{V} = \alpha x^2 + \beta|u|^2$

ABCs FOR A POTENTIAL  $V(x, t)$

$$ABC_1^4 : \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left( e^{-i\mathcal{V}} u \right) + i \frac{\partial_{\mathbf{n}} V}{4} e^{i\mathcal{V}} I_t \left( e^{-i\mathcal{V}} u \right) = 0$$

$$\widetilde{ABC}_2^4 : \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + V} u + \frac{1}{4} \partial_{\mathbf{n}} V (i\partial_t + V)^{-1} u = 0$$

with the phase function:  $\mathcal{V}(x, t) = \int_0^t V(x, s) ds$

NONLINEARITY  $f(u) = g(|u|^2)$

- Cubic  $f(u) = q|u|^2$  / quintic  $f(u) = q|u|^4$
- $f(u) = n_2|u|^2 + n_4|u|^4$ ,  $f(u) = \frac{|u|^2}{1+\sigma|u|^2}$
- Mixed:  $\mathcal{V} = \alpha x^2 + \beta|u|^2$

### ABCs FOR A NONLINEARITY

$$NLABC_1^4 : \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left( e^{-i\mathcal{V}} u \right) + i \frac{\partial_{\mathbf{n}} f(u)}{4} e^{i\mathcal{V}} I_t \left( e^{-i\mathcal{V}} u \right) = 0$$

$$\widetilde{NLABC}_2^4 : \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + f(u)} u + \frac{1}{4} \partial_{\mathbf{n}} f(u) (i\partial_t + f(u))^{-1} u = 0$$

New phase function:  $\mathcal{V}(x, t, u) = \int_0^t f(x, u(x, s)) ds$

PROPOSITION ( $NLABC_1^2$ )

Let  $u_0 \in L^2(\Omega)$  be compactly supported in  $\Omega$ , and let  $f \in C(\mathbb{R}; \mathbb{R})$ .

Assume that there exists a solution  $u \in C^1([0; T[; H^1(\Omega))$  of the problem:

$$\begin{cases} i\partial_t u + \partial_x^2 u + f(u)u = 0, & \text{in } \Omega_T, \\ \partial_n u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} (e^{-i\mathcal{V}} u) = 0, & \text{on } \Sigma_T, \\ u(x, 0) = u_0(x), & \text{on } \Omega, \end{cases} \quad (1)$$

where  $\mathcal{V}(x, t, u) = \int_0^t f(x, u)(x, s) ds$ .

Then,  $u$  satisfies:

$$\forall t > 0, \quad \|u(t)\|_{L^2(\Omega)} \leq \|u_0\|_{L^2(\Omega)}.$$



## DURÀN-SANZ-SERNA SCHEME

$$i \frac{u^{n+1} - u^n}{\Delta t} + \partial_x^2 \frac{u^{n+1} + u^n}{2} + f\left(\frac{u^{n+1} + u^n}{2}\right) \frac{u^{n+1} + u^n}{2} = 0$$

## SCHEME

$$\begin{cases} \frac{2i}{\Delta t} v^{n+1} + \partial_x^2 v^{n+1} + f(v^{n+1}) v^{n+1} = \frac{2i}{\Delta t} u^n, & \text{on } \Omega_T, \\ \partial_{\mathbf{n}} v^{n+1} + \Lambda_p^{M, n+1} v^{n+1} = 0, & \text{on } \Sigma_T, \quad p = 1, 2, \\ + \text{I.C.} \end{cases}$$

with  $v^{n+1} = u^{n+1/2} = \frac{u^{n+1} + u^n}{2}$ .

## DISCRETIZED ABC

- discrete convolution (gauge change)
- or Padé approximants (direct method)

- **PRINCIPLE:** Solve the equation  $i\partial_t u + \Delta u + f(u)u = 0$  through the resolution of the system:

$$\begin{cases} i\partial_t u + \Delta u + \Upsilon u = 0, & \text{on } \Omega_T, \\ \Upsilon = f(u), & \text{on } \Omega_T. \end{cases}$$

- **SEMI DISCRETIZATION**

$$\begin{cases} i \frac{u^{n+1} - u^n}{\Delta t} + \Delta u^{n+1/2} + \Upsilon^{n+1/2} u^{n+1/2} = 0, \\ \frac{\Upsilon^{n+3/2} + \Upsilon^{n+1/2}}{2} = f(u^{n+1}), \end{cases} \quad \text{for } 0 \leq n \leq N$$

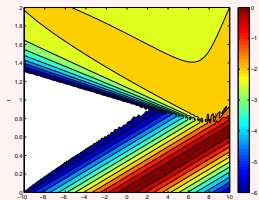
where  $\Upsilon^{n+1/2} = \frac{\Upsilon^{n+1} + \Upsilon^n}{2}$ ,  $\Upsilon^{-1/2} = \Upsilon^{1/2} = f(u^0)$ .

- **INTERESTS :** Speed: equivalent to one fixed point iteration  
Simplicity: same code as for a space- and time-  
depending potential  $V(\mathbf{x}, t)$   
Preservation of the invariants: mass, energy

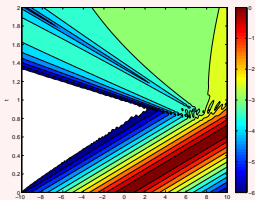
# CUBIC POTENTIAL $\mathcal{V} = q|u|^2$

Initial datum  $u_0 = \sqrt{\frac{2a}{q}} \cdot \text{sech}(\sqrt{a}x) \exp(i\frac{c}{2}x)$  (**soliton**) with  $q = 1$ ,  $a = 2$ ,  $c = 15$

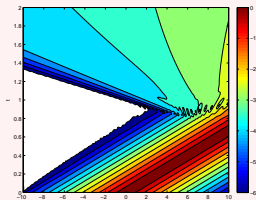
$\Omega_T = [-10; 10] \times [0; 2]$ ,  $\Delta x = 5 \cdot 10^{-3}$ ,  $\Delta t = 10^{-3}$ , 50 Padé functions



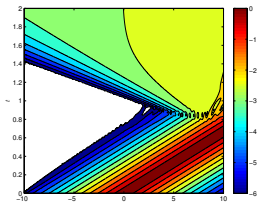
$ABC_0$



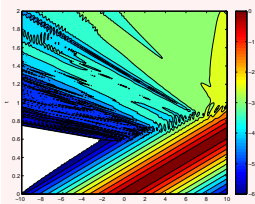
$NLABC_1^2$



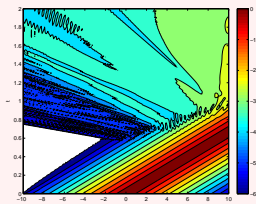
$NLABC_1^4$



PML

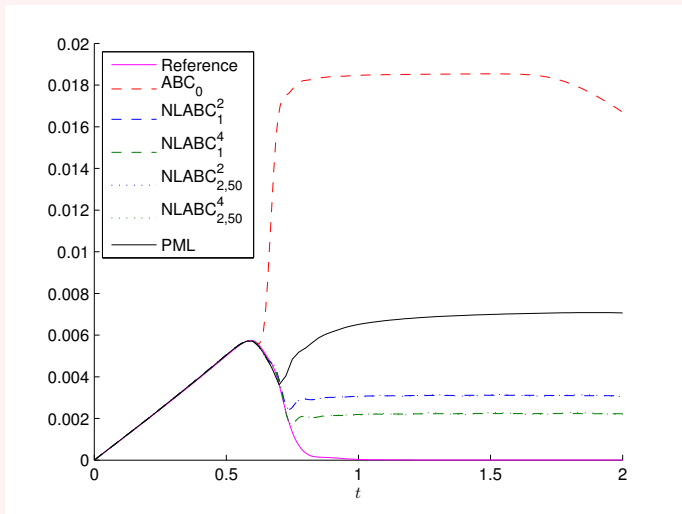


$NLABC_2^2$



$NLABC_2^4$

# RELATIVE $L^2$ ERROR FOR $\mathcal{V} = |u|^2$



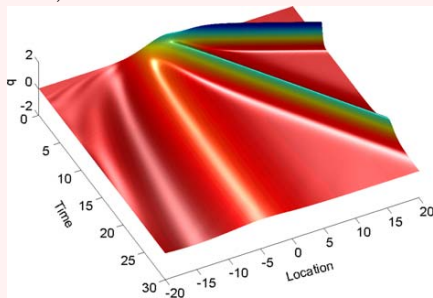
Relative  $L^2$  error  $\frac{\|u(t) - u_{ex}(t)\|_{L^2(\Omega)}}{\|u_{ex}(t)\|_{L^2(\Omega)}}$  for linear and nonlinear ABCs

- Schrödinger : Szeftel (06) (paradifferential technique), Zheng (06) : use of inverse scattering for cubic NLS, exact TBC
- modified KdV : Zheng (06)

$$u_t \pm 6u^2 u_x + u_{xxx} = 0$$

Use of inverse scattering to get exact TBC.

Example (Zheng) : solitary waves generated by an initial Gaussian profile  $u_0(x) = \exp(-1.5x^2)$ .



## SCHRÖDINGER 2D

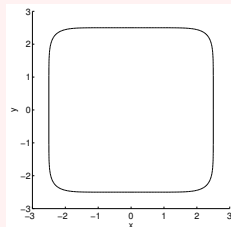
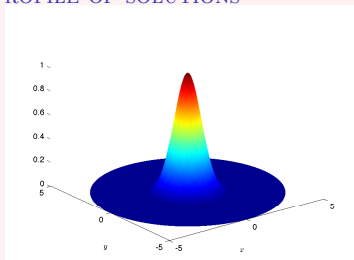
$$\begin{cases} i\partial_t u + \partial_x^2 u + \partial_y^2 u + V(x, y, t) u = 0, & (x, y) \in \mathbb{R}^2, t > 0 \\ u(x, y, 0) = u_0(x, y), & (x, y) \in \mathbb{R}^2 \end{cases}$$

with  $\text{Supp}(u_0) \subset \Omega$ .

$\mathcal{V} = V(t)$ : GAUGE CHANGE

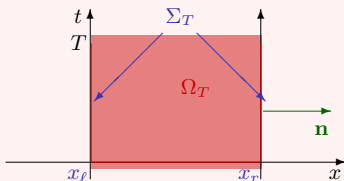
Setting  $\mathcal{V}(t) = \int_0^t V(s) ds$  and  $v(x, y, t) = e^{-i\mathcal{V}(t)} u(x, y, t)$ ,  
then  $v$  is solution of  $i\partial_t v + \partial_x^2 v + \partial_y^2 v = 0$ .

PROFILE OF SOLUTIONS



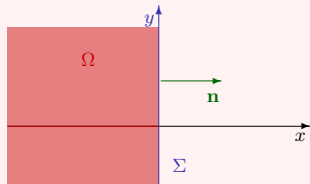
## IN ONE DIMENSION OF SPACE

- Domain  $\Omega_T = [x_\ell; x_r] \times [0; T]$
- Boundary  $\Sigma = \{x_\ell; x_r\}$
- Outwardly directed normal  $\mathbf{n}$  directed according to  $x$
- Fourier transform w.r.t.  $t$  ( $x$  fixed)



## IN DIMENSION TWO WITH STRAIGHT BOUNDARY

- Domain: half-plane  $\Omega = \{x < 0\}$
- Normal  $\mathbf{n}$  directed according to  $x$
- Partial Fourier transform w.r.t.  $(t, y)$  ( $x$  fixed)



$$\partial_x^2 + i\partial_t + \partial_y^2 = 0$$

$i\partial_t + \partial_y^2$  plays the role of  $i\partial_t$  in 1D

$\partial_x^2$  plays the role of  $\partial_x^2$

## FACTORIZATION

- 1D without potential:  $\partial_x^2 + i\partial_t = (\partial_n + i\sqrt{i\partial_t})(\partial_n - i\sqrt{i\partial_t})$
- 1D with variable potential:  
 $\partial_x^2 + i\partial_t + V = (\partial_n + i\sqrt{i\partial_t + V})(\partial_n - i\sqrt{i\partial_t + V}) + R$
- 2D with straight boundary:

$$\partial_x^2 + i\partial_t + \partial_y^2 + V = \left( \partial_n + i\sqrt{i\partial_t + \partial_y^2 + V} \right) \left( \partial_n - i\sqrt{i\partial_t + \partial_y^2 + V} \right) + R$$

TRANSPARENT BOUNDARY CONDITION when  $V|_{\{x \geq 0\}} = 0$ :

$$\partial_n u - i\sqrt{i\partial_t + \partial_y^2} u = 0, \quad \text{on } \Sigma_T.$$



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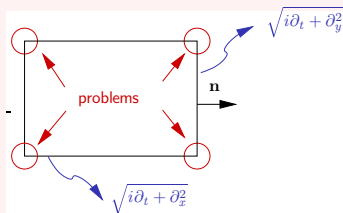
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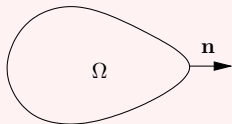
$$\partial_n u - i\sqrt{i\partial_t + \partial_y^2} u = 0, \quad \text{on } \Sigma_T.$$

BOUNDED DOMAIN WITH STRAIGHT BOUNDARY:

Singularities caused by corners



- **CONSIDERATION OF THE GEOMETRY:** convex domain of general, smooth boundary; curvature  $\kappa$ .



- **LOCAL PARAMETRIZATION** of the boundary  
normal variable  $r$ , curvilinear abscissa  $s$

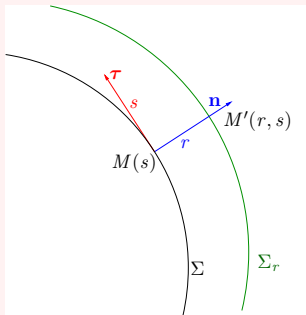
$$\Delta = \partial_r^2 + \kappa_r \partial_r + h^{-1} \partial_s (h^{-1} \partial_s)$$

$\kappa_r = h^{-1} \kappa$ : curvature on the parallel surface  $\Sigma_r$  to  $\Sigma$

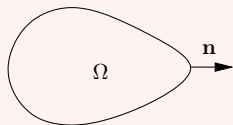
$$h(r, s) = 1 + r\kappa$$

$$L = i\partial_t + \Delta + V$$

$$\Rightarrow L = \partial_r^2 + i\partial_t + \kappa_r \partial_r + h^{-1} \partial_s (h^{-1} \partial_s) + V$$



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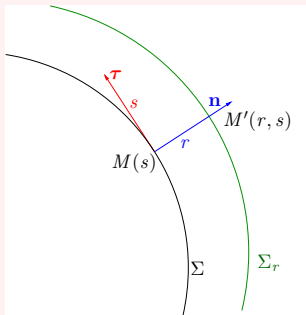
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$$L = \partial_x^2 + i\partial_t + \partial_y^2 + V$$



- Partial Fourier transform w.r.t.  $(s, t)$ ; covariables  $(\xi, \tau)$

$u(\mathbf{r}, \mathbf{s}, t)$ 

- Pseudodifferential operator  $P(\mathbf{r}, \mathbf{s}, t, \partial_{\mathbf{s}}, \partial_t)$  defined through its total symbol  $p(\mathbf{r}, \mathbf{s}, t, \xi, \tau)$  in Fourier space for  $\mathcal{F}_{(\mathbf{s}, t)}$  ( $\xi$  and  $\tau$  covariables of  $\mathbf{s}$  and  $t$ )

$$\begin{aligned} P(\mathbf{r}, \mathbf{s}, t, \partial_{\mathbf{s}}, \partial_t)u(\mathbf{r}, \mathbf{s}, t) &= \mathcal{F}_{(\mathbf{s}, t)}^{-1} \left( p(\mathbf{r}, \mathbf{s}, t, \xi, \tau) \hat{u}(\mathbf{r}, \xi, \tau) \right) \\ &= \int_{\mathbb{R}} \int_{\mathbb{R}} p(\mathbf{r}, \mathbf{s}, t, \xi, \tau) \hat{u}(\mathbf{r}, \xi, \tau) e^{i\mathbf{s}\xi} e^{it\tau} d\xi d\tau \end{aligned}$$

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- Composition rule:  $\sigma(AB) \sim \sum_{|\alpha|=0}^{+\infty} \frac{(-i)^{|\alpha|}}{\alpha!} \partial_{(\xi, \tau)}^{\alpha} \sigma(A) \partial_{(\mathbf{s}, t)}^{\alpha} \sigma(B)$
- Homogeneity according to the couple  $(\xi^2, \tau)$ :  $\sqrt{-\tau - \xi^2}$  is of order 1

Order  $m$ :  $f(\mathbf{r}, \mathbf{s}, t, \lambda\xi, \lambda^2\tau) = \lambda^m f(\mathbf{r}, \mathbf{s}, t, \xi, \tau)$

- Asymptotic expansion in homogeneous symbols:  $P \in OPS^m$  if:

$$p(\mathbf{r}, \mathbf{s}, t, \xi, \tau) \sim \sum_{j=0}^{+\infty} p_{m-j}(\mathbf{r}, \mathbf{s}, t, \xi, \tau),$$

where  $p_{m-j}$  is homogeneous of order  $m - j$ ;  $p_m$  is the principal symbol.

## 1 - GAUGE CHANGE

- Change of unknown (which solve the case  $\mathcal{V} = V(t)$ )

$$v = e^{-i\mathcal{V}}u \quad \text{avec} \quad \mathcal{V}(r, s, t) = \int_0^t V(r, s, \sigma) d\sigma$$

- We work on the equation written for  $v$ :

$$i\partial_t v + \partial_r^2 v + (\kappa_r + F)\partial_r v + h^{-1}\partial_s(h^{-1}\partial_s v) + G v = 0$$

## 2 - DIRECT METHOD

- We work directly on the original equation (with local coordinates)

$$i\partial_t u + \partial_r^2 u + \kappa_r \partial_r u + h^{-1}\partial_s(h^{-1}\partial_s u) + V u = 0$$

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⇒ Absorbing boundary condition for

$$Lw = i\partial_t w + \partial_r^2 w + (\kappa_r + A)\partial_r w + h^{-1}\partial_s(h^{-1}\partial_s w) + Bw = 0, \quad \text{with}$$

- $A = F(r, s, t)$  and  $B = G(r, s, t)$  if  $w = v = e^{-i\mathcal{V}}u$
- $A = 0$  and  $B = V(r, s, t)$  if  $w = u$ ,

## UNIFICATION OF BOTH STRATEGIES: General Schrödinger operator:

$$L = i\partial_t + \partial_r^2 + (\kappa_r + A)\partial_r + h^{-1}\partial_s(h^{-1}\partial_s) + B$$

### FACTORIZATION OF NIRENBERG-TYPE OF OPERATOR $L$

$$L = (\partial_r + i\Lambda^-)(\partial_r + i\Lambda^+) + R \quad \text{on } \Sigma_r,$$

where :

$\Lambda^\pm(r, s, t, \partial_s, \partial_t) \in OPS^1$  is a pseudodifferential operator of order 1,

$R \in OPS^{-\infty}$ ,

and  $\Lambda^+$  admits the asymptotic expansion in homogeneous symbols:

$$\sigma(\Lambda^+) = \lambda^+ \sim \sum_{j=0}^{+\infty} \lambda_{1-j}^+ = \lambda_1^+ + \lambda_0^+ + \lambda_{-1}^+ + \lambda_{-2}^+ + \dots$$

with  $\lambda_{1-j}^+$  homogeneous of order  $1 - j$  according to the couple  $(\xi^2, \tau)$ .

The knowledge of the symbols  $(\lambda_j^+)$  describes entirely the operator  $\Lambda^+$ .

BACK ON THE SURFACE  $\Sigma$ :

$$\widetilde{\Lambda}^+ = \Lambda^+|_{r=0}$$

$$\widetilde{\lambda}_j = (\lambda_j^+)|_{r=0}$$



ABSORBING BOUNDARY CONDITION which expresses that the wave is outgoing:

$$\partial_{\mathbf{n}} w + i \widetilde{\Lambda}^+ w = 0 \quad \text{where} \quad \widetilde{\Lambda}^+ = Op \left( \sum_{j=0}^{+\infty} \widetilde{\lambda}_{1-j} \right)$$

$$\partial_{\mathbf{n}} w + i \sum_{j=0}^{+\infty} Op \left( \widetilde{\lambda}_{1-j} \right) w = 0, \quad \text{on } \Sigma_T$$

IDENTIFICATION OF THE PRINCIPAL SYMBOL  $\lambda_1^+$

Outgoing wave  $\text{Im}(\lambda_1^+(s, t, \xi, \tau)) \leq 0$ , for  $|\tau| \gg 1$

$$\text{Strategy 1} \quad \lambda_1^+ = -\sqrt{-\tau - h^{-2}\xi^2}$$

$$\text{Strategy 2} \quad \lambda_1^+ = -\sqrt{-\tau - h^{-2}\xi^2 + ih^{-1}(\partial_s h^{-1})\xi + V}$$

Asymptotic expansion:  $\widetilde{\lambda}_j$  are functions of  $\sqrt{-\tau - \xi^2}$  (resp.  $\sqrt{-\tau - \xi^2 + V}$ ).

$\implies$  non local operators w.r.t to time AND space

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$$\partial_{\mathbf{n}} w_M + i \sum_{j=0}^{M-1} Op \left( \widetilde{\lambda}_{1-j} \right) w_M = 0, \quad \text{on } \Sigma_T$$

Approximate condition of order  $M$

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$\Rightarrow$  non local operators w.r.t to time AND space

Approach valid for both strategies.

- Taylor expansion of the symbols, under the assumption  $|\tau| \gg \xi^2$ .

$$-\tau - \xi^2 + b = -\tau \left( 1 + \frac{\xi^2}{\tau} - \frac{b}{\tau} \right)$$

Thereby:

$$\sqrt{-\tau - \xi^2 + b} \approx \sqrt{-\tau} \left( 1 + \frac{\xi^2}{2\tau} - \frac{b}{2\tau} \right) = \sqrt{-\tau} - \frac{\xi^2}{2} \frac{1}{\sqrt{-\tau}} + \frac{b}{2} \frac{1}{\sqrt{-\tau}}$$

- Then

$$Op(\sqrt{-\tau}) = e^{i\pi/4} \partial_t^{1/2},$$

$$Op(\xi) = -i\partial_s,$$

$$Op\left(\frac{1}{\sqrt{-\tau}}\right) = e^{-i\pi/4} I_t^{1/2},$$

$$Op(\xi^2) = -\partial_s^2 = -\Delta_\Sigma,$$

$$Op\left(\frac{1}{\tau}\right) = i I_t$$

$\implies$  The operators are localized in space only

We approximate  $ABC_2^1$  (direct method) :  $\partial_{\mathbf{n}}u - i\sqrt{i\partial_t + \Delta_{\Sigma} + V}u = 0$ , on  $\Sigma_T$ .

## PADÉ APPROXIMANTS OF ORDER $m$

$$\sqrt{z} \approx R_m(z) = \sum_{k=1}^m \frac{a_k^m z}{z + d_k^m} = \sum_{k=0}^m a_k^m - \sum_{k=1}^m \frac{a_k^m d_k^m}{z + d_k^m}$$

$ABC_2^1$  becomes  $ABC_{2,P}^1$  :  $\partial_{\mathbf{n}}u - i R_m(i\partial_t + \Delta_{\Sigma} + V)u = 0$

$$\partial_{\mathbf{n}}u - i \left( \sum_{k=0}^m a_k^m \right) u + i \sum_{k=1}^m a_k^m d_k^m \underbrace{(i\partial_t + \Delta_{\Sigma} + V + d_k^m)^{-1}}_{\varphi_k} u = 0$$

We introduce  $m$  auxiliary functions defined on  $\Sigma$

$$(i\partial_t + \Delta_{\Sigma} + V + d_k^m)\varphi_k = u, \quad 1 \leq k \leq m$$

We get a coupling between  $u$  and  $(\varphi_k)_{1 \leq k \leq m}$  on  $\Sigma$

$$\begin{cases} \left( \sum_{k=0}^m a_k^m \right) u - \sum_{k=1}^m a_k^m d_k^m \varphi_k \\ i\partial_t \varphi_k + \Delta_{\Sigma} \varphi_k + (V + d_k^m) \varphi_k = u, \quad 1 \leq k \leq m. \end{cases}$$

$\Rightarrow$  The operators are localized in space AND time

- GAUGE CHANGE

$$\begin{aligned}
 \text{ABC}_{1,T}^2 & \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left( e^{-i\mathcal{V}} u \right) + \frac{\kappa}{2} u \\
 \text{ABC}_{1,T}^3 & \quad - e^{i\pi/4} e^{i\mathcal{V}} \left( \frac{\kappa^2}{8} + \frac{\Delta_{\Sigma}}{2} + i\partial_s \mathcal{V} \partial_s + \frac{1}{2} (i\partial_s^2 \mathcal{V} - (\partial_s \mathcal{V})^2) \right) I_t^{1/2} \left( e^{-i\mathcal{V}} u \right) \\
 \text{ABC}_{1,T}^4 & \quad + i e^{i\mathcal{V}} \left( \frac{\partial_s (\kappa \partial_s)}{2} + \frac{\kappa^3 + \partial_s^2 \kappa}{8} + \frac{i\partial_s \kappa \partial_s \mathcal{V}}{2} \right) I_t \left( e^{-i\mathcal{V}} u \right) \\
 & \quad - i \frac{\text{sg}(\partial_{\mathbf{n}} V)}{4} \sqrt{|\partial_{\mathbf{n}} V|} e^{i\mathcal{V}} I_t \left( \sqrt{|\partial_{\mathbf{n}} V|} e^{-i\mathcal{V}} u \right) = 0
 \end{aligned}$$

- DIRECT METHOD

$$\begin{aligned}
 \text{ABC}_{2,T}^2 & \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} \partial_t^{1/2} u + \frac{\kappa}{2} u \\
 \text{ABC}_{2,T}^3 & \quad - e^{i\pi/4} \left( \frac{\kappa^2}{8} + \frac{\Delta_{\Sigma}}{2} \right) I_t^{1/2} u - e^{i\pi/4} \frac{\text{sg}(V)}{2} \sqrt{|V|} I_t^{1/2} \left( \sqrt{|V|} u \right) \\
 \text{ABC}_{2,T}^4 & \quad + i \left( \frac{\partial_s (\kappa \partial_s)}{2} + \frac{\kappa^3 + \partial_s^2 \kappa}{8} \right) I_t u - i \frac{\text{sg}(\partial_{\mathbf{n}} V)}{4} \sqrt{|\partial_{\mathbf{n}} V|} I_t \left( \sqrt{|\partial_{\mathbf{n}} V|} u \right) = 0
 \end{aligned}$$

- GAUGE CHANGE

$$\begin{aligned}
 \text{ABC}_{1,P}^1 & \quad \partial_{\mathbf{n}} u - i e^{i\mathcal{V}} \sqrt{i\partial_t + \Delta_{\Sigma}} \left( e^{-i\mathcal{V}} u \right) \\
 \text{ABC}_{1,P}^2 & \quad + \frac{\kappa}{2} u + \partial_s \mathcal{V} e^{i\mathcal{V}} \partial_s (i\partial_t + \Delta_{\Sigma})^{-1/2} \left( e^{-i\mathcal{V}} u \right) \\
 & \quad - \frac{\kappa}{2} e^{i\mathcal{V}} (i\partial_t + \Delta_{\Sigma})^{-1} \Delta_{\Sigma} \left( e^{-i\mathcal{V}} u \right) = 0
 \end{aligned}$$

- DIRECT METHOD

$$\begin{aligned}
 \text{ABC}_{2,P}^1 & \quad \partial_{\mathbf{n}} u - i \sqrt{i\partial_t + \Delta_{\Sigma} + V} u \\
 \text{ABC}_{2,P}^2 & \quad + \frac{\kappa}{2} u - \frac{\kappa}{2} (i\partial_t + \Delta_{\Sigma} + V)^{-1} \Delta_{\Sigma} u = 0
 \end{aligned}$$

For conditions  $ABC_{1,T}^M$  and  $ABC_{2,T}^M$  (Taylor)

### PROPOSITION

Let  $u_0 \in L^2(\Omega)$  s.t.  $\text{Supp}(u_0) \subset \Omega$ . Let  $V \in C^\infty(\mathbb{R}^2 \times \mathbb{R}^+, \mathbb{R})$  and  $u$  a solution of

$$\begin{cases} i\partial_t u + \partial_x^2 u + Vu = 0, & \text{in } \Omega_T, \\ \partial_n u + \Lambda_{j,T}^M u = 0, & \text{on } \Sigma_T, \quad j = 1, 2, \\ u(x, 0) = u_0(x), & \forall x \in \Omega. \end{cases}$$

We assume that we are in the quasi-hyperbolic area  $\mathcal{H} = \{-\tau - \xi^2 > 0\}$ .

Then,  $u$  fulfills the following energy bound

$$\forall t > 0, \quad \|u(t)\|_{L^2(\Omega)} \leq \|u_0\|_{L^2(\Omega)}, \quad (\text{E1})$$

- for  $M = 2$ ,
- for  $M = 3$  if  $V$  is positive on  $\Sigma$  ( $ABC_{2,T}^3$ ) or if  $V$  and  $\Omega$  are radially symmetrical ( $ABC_{1,T}^3$ ),
- for  $M = 4$  if  $\partial_n V$  is of constant sign on  $\Sigma$ , and if furthermore  $\partial_n V$  is positive on  $\Sigma$  ( $ABC_{2,T}^4$ ) or if the problem is radially symmetrical ( $ABC_{1,T}^4$ ),

which implies the uniqueness of the solution.

Time step  $\Delta t = T/N$ ,  $t_n = n\Delta t$ ,  
 $u^n(r, s) \approx u(r, s, t_n)$  for  $0 \leq n \leq N$ .

### INTERIOR EQUATION:

Semi discrete Crank-Nicolson scheme: symmetrical, unconditionally stable

$$i \frac{u^{n+1} - u^n}{\Delta t} + \Delta \frac{u^{n+1} + u^n}{2} + \frac{V^{n+1} + V^n}{2} \frac{u^{n+1} + u^n}{2} = 0$$

for  $n = 0, \dots, N - 1$ .

### IMPLEMENTATION:

$$\frac{2i}{\Delta t} v^{n+1} + \Delta v^{n+1} + V^{n+1/2} v^{n+1} = \frac{2i}{\Delta t} u^n$$

with  $v^{n+1} = u^{n+1/2} = \frac{u^{n+1} + u^n}{2}$ ,  $V^{n+1/2} = \frac{V^{n+1} + V^n}{2}$ .

### SPACE DISCRETIZATION : Finite Element Method



$$ABC_{1,T}^2 : \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left( e^{-i\mathcal{V}} u \right) + \frac{\kappa}{2} u = 0, \quad \text{on } \Sigma_T$$

$$\partial_{\mathbf{n}} v^{n+1} + e^{-i\pi/4} e^{i\mathcal{W}^{n+1}} \sqrt{\frac{2}{\Delta t}} \sum_{k=0}^{n+1} \beta_{n+1-k} e^{-i\mathcal{W}^k} v^k + \frac{\kappa}{2} v^{n+1} = 0, \quad n \geq 0.$$

$$\partial_{\mathbf{n}} v^{n+1} + \left( e^{-i\pi/4} \beta_0 + \frac{\kappa}{2} \right) v^{n+1} + e^{-i\pi/4} e^{i\mathcal{W}^{n+1}} \sqrt{\frac{2}{\Delta t}} \sum_{k=0}^n \beta_{n+1-k} e^{-i\mathcal{W}^k} v^k = 0.$$

## PROPOSITION

For discretized boundary conditions  $ABC_{1,T}^M$  or  $ABC_{2,T}^M$ , we have

$$\forall n \in \{0, \dots, N\}, \quad \|u^n\|_{L^2(\Omega)} \leq \|u^0\|_{L^2(\Omega)}, \quad (2)$$

under the semi discrete assumptions equivalent to those of the continuous case.

The unconditional stability of the scheme is preserved.

System associated to the boundary condition  $ABC_{2,P}^1$ :

$$\partial_{\mathbf{n}} u - i\sqrt{i\partial_t + \Delta_{\Sigma} + V} u = 0$$

$$\left\{ \begin{array}{l} i\partial_t u + \Delta u + V u = 0, \quad \text{on } \Omega_T, \\ \partial_{\mathbf{n}} u - i \left( \sum_{k=0}^m a_k^m \right) u + i \sum_{k=0}^m a_k^m d_k^m \varphi_k = 0, \quad \text{on } \Sigma_T, \\ (i\partial_t + \Delta_{\Sigma} + V + d_k^m) \varphi_k = u, \quad \text{on } \Sigma_T, \quad \text{pour } 1 \leq k \leq m. \end{array} \right.$$

CRANK-NICOLSON SCHEME ( $m + 1$  EQUATIONS):

$$\left\{ \begin{array}{l} \frac{2i}{\Delta t} u^{n+1/2} + \Delta u^{n+1/2} + V^{n+1/2} u^{n+1/2} = \frac{2i}{\Delta t} u^n, \quad \text{on } \Omega, \\ \partial_{\mathbf{n}} u^{n+1/2} - i \left( \sum_{k=0}^m a_k^m \right) u^{n+1/2} + i \sum_{k=0}^m a_k^m d_k^m \varphi_k^{n+1/2} = 0, \quad \text{on } \Sigma, \\ \frac{2i}{\Delta t} \varphi_k^{n+1/2} + \Delta_{\Sigma} \varphi_k^{n+1/2} + V^{n+1/2} \varphi_k^{n+1/2} + d_k^m \varphi_k^{n+1/2} = u^{n+1/2} + \frac{2i}{\Delta t} \varphi_k^n, \quad \text{on } \Sigma. \end{array} \right.$$

- System in  $(u^{n+1/2}, \varphi_1^{n+1/2}, \dots, \varphi_m^{n+1/2})$ , coupled through the boundary  $\Sigma$ .
- Entirely local / No stability result

# NUMERICAL EXAMPLES

Initial datum:  $u_0(x, y) = e^{-(x^2+y^2)-ik_0x}$ ,  
with  $k_0 = 10$

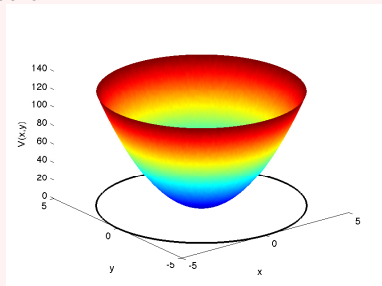
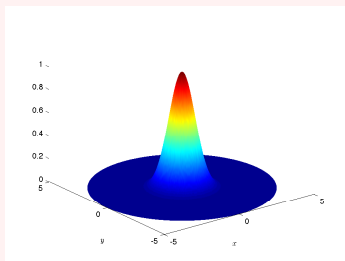
$\Delta t = 10^{-3}$ ,  $T = 1$

Disk meshed with 1 700 000 triangles

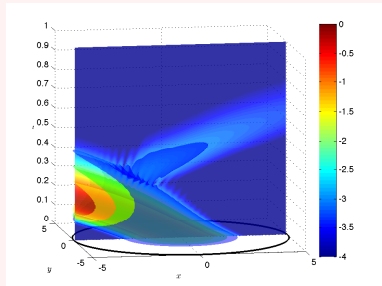
25 Padé functions

Logarithmic levels, threshold  $10^{-4}$

**DOMAINS:** disk / mediator / “smoothed square”



POTENTIAL ON DISK



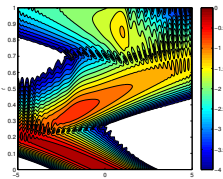
PROFILE OF AN APPROXIMATE  
SOLUTION

$$V(r) = 5r^2$$

$$r = \sqrt{x^2 + y^2}$$

TAYLOR  
PROACH

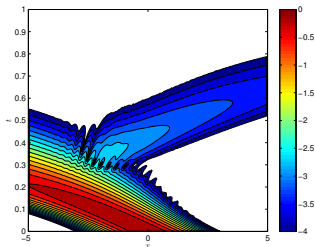
AP-



Condition without  
potential

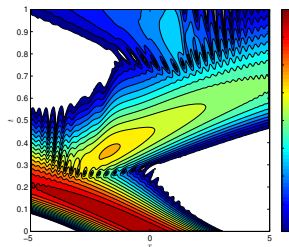
PADÉ APPROACH

GAUGE CHANGE

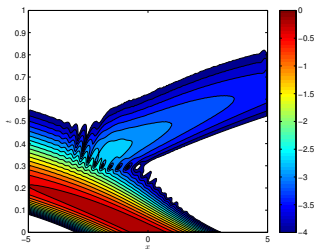


$ABC_{1,T}^4$

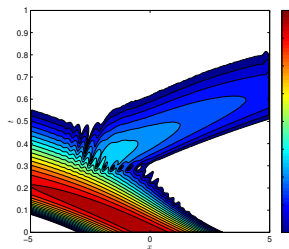
DIRECT METHOD



$ABC_{2,T}^4$

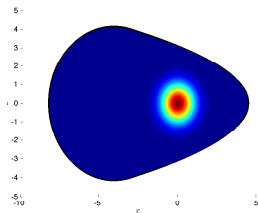


$ABC_{1,P}^2$

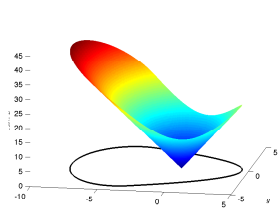


$ABC_{2,P}^2$

## INITIAL DATUM

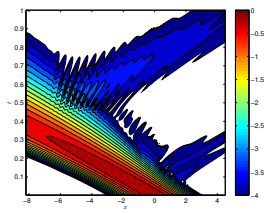


## PROFILE OF THE POTENTIAL

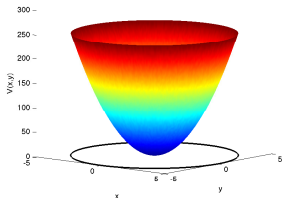
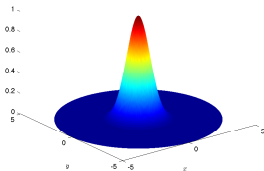


$$V(x, y) = 5\sqrt{x^2 + y^2}$$

## ABC

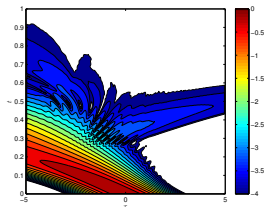


$$ABC_{2,P}^2$$



Potential at  $t = 0$

$$V(x, y, t) = 5(x^2 + y^2)(1 + \cos(4\pi t))$$



$$ABC_{1,T}^4$$

$$\mathcal{V}(x, y, t) = \int_0^t f(u)$$

- TAYLOR APPROACH, GAUGE CHANGE

$$NLABC_{1,T}^2 \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left( e^{-i\mathcal{V}} u \right) + \frac{\kappa}{2} u = 0$$

- TAYLOR APPROACH, DIRECT METHOD

$$NLABC_{2,T}^2 \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} \partial_t^{1/2} u + \frac{\kappa}{2} u$$

$$NLABC_{2,T}^3 \quad - e^{i\pi/4} \left( \frac{\kappa^2}{8} + \frac{\Delta_{\Sigma}}{2} \right) I_t^{1/2} u - e^{i\pi/4} \frac{\text{sg}(f(u))}{2} \sqrt{|f(u)|} I_t^{1/2} \left( \sqrt{|f(u)|} u \right)$$

$$NLABC_{2,T}^4 \quad + i \left( \frac{\partial_s(\kappa \partial_s)}{2} + \frac{\kappa^3 + \partial_s^2 \kappa}{8} \right) I_t u$$

$$- i \frac{\text{sg}(\partial_{\mathbf{n}} f(u))}{4} \sqrt{|\partial_{\mathbf{n}} f(u)|} I_t \left( \sqrt{|\partial_{\mathbf{n}} f(u)|} u \right) = 0$$

- PADÉ APPROACH, DIRECT METHOD

$$NLABC_{2,P}^1 \quad \partial_{\mathbf{n}} u - i \sqrt{i \partial_t + \Delta_{\Sigma} + f(u)} u$$

$$NLABC_{2,P}^2 \quad + \frac{\kappa}{2} u - \frac{\kappa}{2} (i \partial_t + \Delta_{\Sigma} + f(u))^{-1} \Delta_{\Sigma} u = 0$$

## FIXED POINT METHOD

- Interior equation: Duràn - Sanz-Serna scheme

$$i \frac{u^{n+1} - u^n}{\Delta t} + \Delta \frac{u^{n+1} + u^n}{2} + f\left(\frac{u^{n+1} + u^n}{2}\right) \frac{u^{n+1} + u^n}{2} = 0$$

- Energy bound:  $\|u^n\|_{L^2(\Omega)} \leq \|u^0\|_{L^2(\Omega)}$ 
  - for  $NLABC_{2,T}^2$  and  $NLABC_{1,T}^2$
  - for  $NLABC_{2,T}^3$  when  $f(u) \geq 0$ .

## RELAXATION METHOD

- 

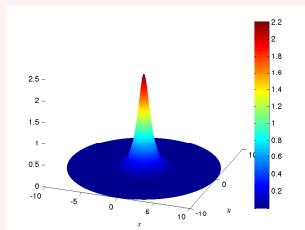
$$\begin{cases} i \frac{u^{n+1} - u^n}{\Delta t} + \Delta u^{n+1/2} + \Upsilon^{n+1/2} u^{n+1/2} = 0, \\ \frac{\Upsilon^{n+3/2} + \Upsilon^{n+1/2}}{2} = f(u^{n+1}), \end{cases} \quad \text{for } 0 \leq n \leq N$$

with  $\Upsilon^{n+1/2} = \frac{\Upsilon^{n+1} + \Upsilon^n}{2}$ ,  $\Upsilon^{-1/2} = f(u^0)$ .

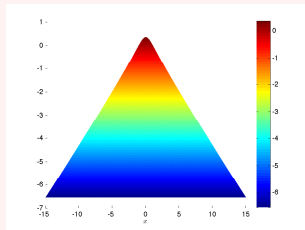
- Cubic equation  $i\partial_t + \Delta u + q|u|^2u = 0$
- Numerical construction of the soliton: the search of stationary solutions leads to

$$\begin{cases} \partial_r^2 \psi + \frac{1}{r} \partial_r \psi - \psi + q|\psi|^2 \psi = 0, & 0 < r < R, \\ \psi'(0) = 0, & \psi(0) = \beta, \end{cases}$$

solved by a shooting method [Di Menza 09]



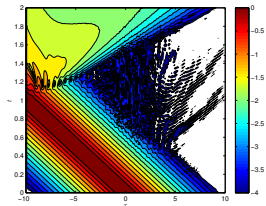
$|u_0|$  on  $R = 10$



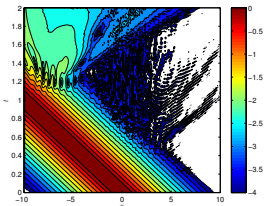
$|u_0|$  in logarithmic scale on  $R = 15$



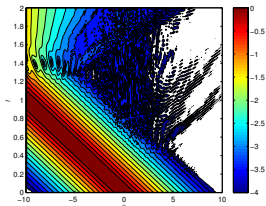
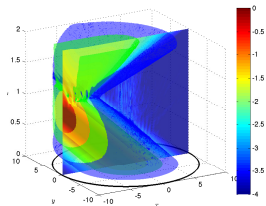
WITHOUT POTENTIAL

 $ABC_0$ 

GAUGE CHANGE

 $NLABC_{1,T}^2$ 

DIRECT METHOD

 $NLABC_{2,T}^3$ 

Initial datum: soliton

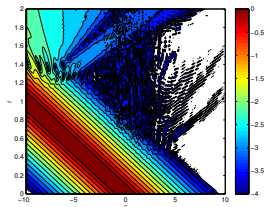
Domain: disc of radius 10

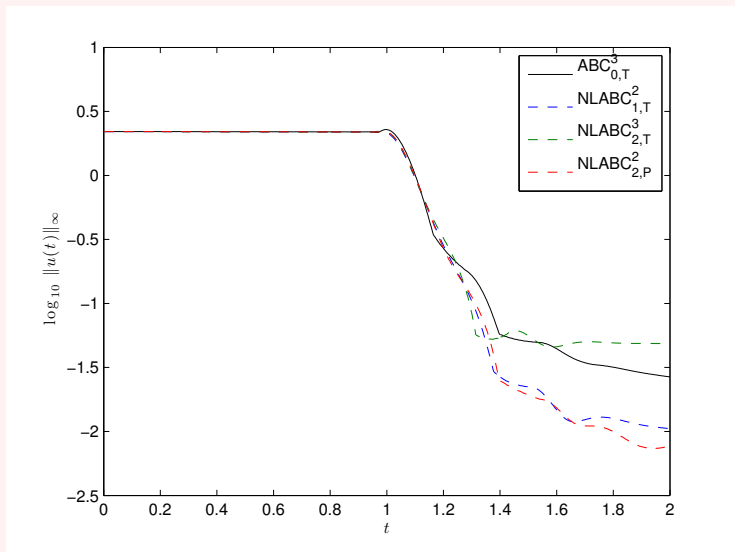
 $\Delta t = 2 \times 10^{-3}$ 

1 700 000 triangles

 $k_0 = 5$  $T = 2$ 

Logarithmic scale

 $NLABC_{2,P}^2$

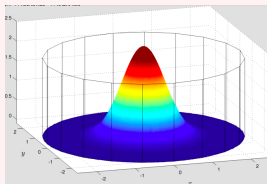


$L^\infty$  norm associated to different ABCs (logarithmic scale)

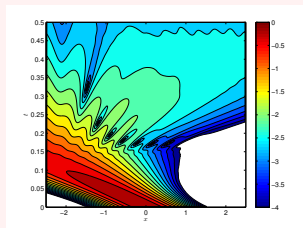
$$u_0(x, y) = e^{-\frac{x^2+y^2}{0.5^2}} - 10ix$$

Circular domain,  $R = 2.5$

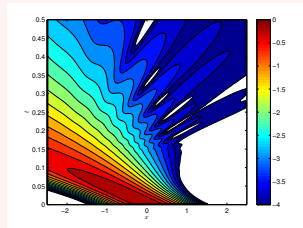
$$\mathcal{V} = |u|^2$$



$$\mathcal{V} = x^2 + y^2 + |u|^2$$



$ABC_0$



$NLABC_{2,P}^2$