

A structure-preserving scheme for the von Neumann equation with singular self-interaction

Numerical investigation of the onset of instability

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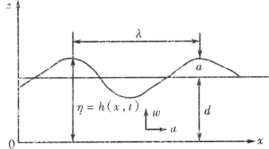
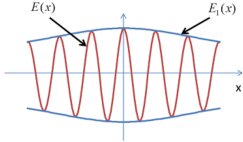


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Outline

- ① A non-standard equation: context and key features
- ② The numerical scheme
- ③ Numerical investigation of the fully nonlinear problem

Ocean waves: many scales, many equations

<p>phase-resolved</p>	<p>full free boundary problem, Serre-Green-Naghdi, Boussinesq, Whitham, ...</p>	
<p>envelope</p>	<p>NLS, crossing seas NLS system, Dysthe, NLS variants, Zakharov, ...</p>	 <p>$E(x) = E_1(x)e^{-i\theta_1 x}$</p>
<p>phase-averaged</p>	<p>Hasselmann / wave kinetic eq., Longuet-Higgins, Alber, Crawford-Saffman-Yuen, ...</p>	<p>> 10km × 10km metocean data lives here</p>

From NLS to the Alber equation

Gravity wave envelope $\eta(x, t) = \text{Re} [\psi(x, t)e^{i(k_0x - \omega_0t)}]$ satisfies NLS:

$$i\partial_t\psi + \frac{p}{2}\Delta\psi + \frac{q}{2}|\psi|^2\psi = 0.$$

Sea states are stationary & homogeneous, characterised by their spectrum $P(k)$:

$$E[\psi(x, t)\bar{\psi}(x', t)] = \Gamma(x - x') + o(1), \quad \mathcal{F}[\Gamma] = P.$$

Via **2nd moments + Gaussian closure + quasi-homogeneity** [Alber, PRSA 1978]: write $R(x, y, t) = \Gamma(x - y) + u(x, y, t)$, to get

$$i\partial_t u + p(\Delta_x - \Delta_y)u + q(u(x, x, t) - u(y, y, t))(\Gamma(x - y) + u) = 0.$$

Alber & von Neumann equations

Denote the inhomogeneity by $u(x, y, t)$, and the **trace nonlinearity**
 $V(x, t) = u(x, x, t)$:

$$i\partial_t u + p(\Delta_x - \Delta_y)u + q\left(V(x, t) - V(y, t)\right) \left(\Gamma(x - y) + u(x, y, t)\right) = 0,$$
$$\mathbf{V(x, t) = \delta_x * u(x, x, t)}, \quad u(x, y, 0) = u_0(x, y).$$

- **Hyperbolic Laplacian:** $\Delta_x - \Delta_y$
- **Nonlocal:** (x, y, t) coupled with (x, x, t) , (y, y, t)
- **Singular kernel, loss of $d/2$ derivatives:** trace operator $u(x, y, t) \mapsto u(x, x, t)$ behaves like a $d/2$ -order differential operator

⇒ Similar to **von Neumann equations** of quantum statistical mechanics; however these typically have smooth interaction kernels.

The bifurcation and marine safety

The full equation can be recast as

$$i\partial_t u + \mathcal{L}_\Gamma u = \mathcal{Q}(u, u).$$

Linear stability of the background Γ :

$$i\partial_t u + \mathcal{L}_\Gamma u = 0$$

- vast majority of metocean data: $P(k) \leftrightarrow \Gamma(x - y)$
- linear stability criterion involves only $P(k)$
[Alber PRSA 1978; A. et al. KRM, 2020; A. arXiv:2604.16998]
- open questions:
how do borderline stable / unstable problems behave?
what can we say about rogue waves?

This talk

- **This paper:** A., Karakatsani & Kyza, arXiv:2506.06879
“A structure-preserving, second-order-in-time scheme for the von Neumann equation with power nonlinearity”
- A relaxation Crank-Nicolson scheme: linearly implicit, $O(\tau^2 + h^4)$
- Structure-preserving: discrete balance law, exact invariants
- The **initialization problem** for Besse-type schemes
- Numerical investigation of the onset of modulation instability
- Monte Carlo for localized extreme events

Building on: [A., Athanassoulis, Ptashnyk & Sapsis, KRM 2020],
[A. & Kyza, Water Waves 2024],
[A., Katsaounis, Kyza, Studies Appl. Math. 2024]

Relaxation Crank-Nicolson scheme

Augmented system with auxiliary variable ϕ :

$$\begin{aligned}\phi(x, y, t) &= u(x, x, t) - u(y, y, t), \\ i\partial_t u + p(\Delta_x - \Delta_y)u + q\phi \left(\Gamma(x - y) + u \right) &= 0.\end{aligned}$$

Time-discrete scheme (inspired by [Besse, SINUM 2004]):

$$\begin{aligned}\frac{1}{2} \left(\Phi^{n+\frac{1}{2}} + \Phi^{n-\frac{1}{2}} \right) &= U^n(x, x) - U^n(y, y), \\ i \frac{U^{n+1} - U^n}{\tau} + p(\Delta_x - \Delta_y)U^{n+\frac{1}{2}} + q\Phi^{n+\frac{1}{2}} \left(\Gamma(x - y) + U^{n+\frac{1}{2}} \right) &= 0\end{aligned}$$

where $U^{n+\frac{1}{2}} := (U^{n+1} + U^n)/2$.

Linearly implicit: only one linear system per timestep.

4th-order finite differences in space; $\Phi^{-1/2}$ **required to start.**

Consistency, boundedness, and balance laws

Consistency: residuals are $O(\tau^2)$ in time and $O(h^4)$ in space.

Boundedness: the total L^2 norm

$$\mathcal{N}^n = \|\Gamma(x - y) + U^n\|_{L^2}^2$$

is conserved at the discrete level, **unconditionally in τ** .

Discrete balance law: if $\mathcal{M}^n := \|U^n\|_{L^2}^2$, then

$$\frac{\mathcal{M}^{n+1} - \mathcal{M}^n}{\tau} = 2 \operatorname{Re} \left[iq \left\langle \Phi^{n+\frac{1}{2}} \Gamma(x - y), U^{n+\frac{1}{2}} \right\rangle \right],$$

reflecting the continuous balance law

$$\frac{d}{dt} \mathcal{M}(t) = 2 \operatorname{Re} \left[iq \left\langle \left(V(x, t) - V(y, t) \right) \Gamma(x - y), u(x, y, t) \right\rangle \right].$$

The initialization problem

The scheme requires $\Phi^{-1/2}$ to start. Two options:

Naive: $\Phi_{i,j}^{-\frac{1}{2}} = U_{i,i}^0 - U_{j,j}^0$.

Advanced (proposed): take a backward half-step:

$$\left\{ \begin{array}{l} \Phi_{i,j}^* = U_{i,i}^0 - U_{j,j}^0, \\ \left(I + i\frac{p\tau}{4}\mathcal{D}_H + i\frac{q\tau}{4}\mathfrak{F}^* \right) \text{vec}(U_{i,j}^{-\frac{1}{4}}) = \text{vec}(U_{i,j}^0 - i\frac{q\tau}{4}\Gamma_{i,j}\Phi_{i,j}^*), \\ \Phi_{i,j}^{-\frac{1}{2}} = (2U_{i,j}^{-\frac{1}{4}} - U_{i,j}^0)|_{\text{diag}}. \end{array} \right.$$

	Naive	Advanced
EOC in space, U and Φ	4	4
EOC in time, U	2	2
EOC in time, Φ	1	2

This issue recurs across Besse-type schemes, e.g.,

[A., Katsaounis, Kyza, *Studies Appl. Math.* 2024; Zouraris, *SINUM* 2023].

Setup for the bifurcation study

Gaussian power spectrum, onset of linear instability at $C_* \approx 0.99$:

$$\mathcal{F}[\Gamma] = P(k) = \frac{C^2}{\sigma} e^{-\pi k^2 / \sigma^2}, \quad \sigma = 0.36, \quad C \in [0.9, 1.9].$$

Initial inhomogeneity (Hermitian, localized):

$$f_0(x, y) = 0.05 \cdot e^{-0.06x^2 - 0.07y^2} (1 + A_1 \cos(0.3x) \cos(0.2y) + A_2x + A_3y),$$
$$u_0 = \frac{1}{2}(f_0 + \overline{f_0}^T), \quad \|u_0\|_{L^2} \approx 0.31, \quad \|u_0\|_{L^\infty} \approx 0.06.$$

Domain: $(x, y) \in [-25, 25]^2$, $\tau = 10^{-3}$, $h = 9 \times 10^{-2}$.

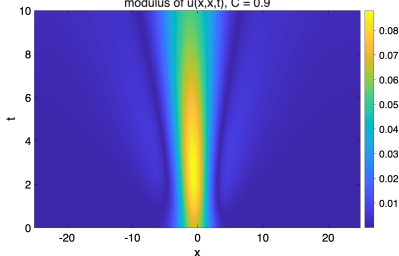
Code: github.com/aathanas/rcn_Alber_MATLAB.

Landau damping vs. modulation instability

$$u(x, x, t) \approx \text{Var}[\psi(x, t)] - \text{Var}[\psi]$$

Stable: $C = 0.9 < C_*$

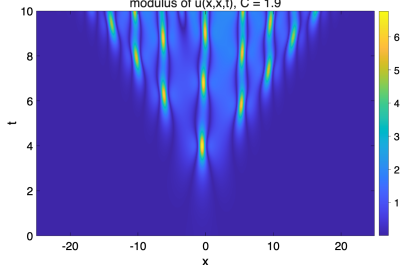
modulus of $u(x, x, t)$, $C = 0.9$



The inhomogeneity disperses.
Values $O(10^{-2} - 10^{-1})$

Unstable: $C = 1.9 > C_*$

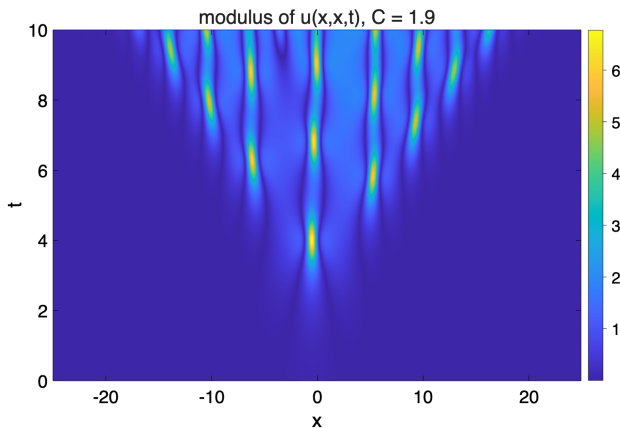
modulus of $u(x, x, t)$, $C = 1.9$



First exponential growth,
then coherent structures.
Values $O(10^0 - 10^1)$

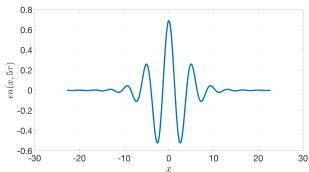
The meta-stable lattice

- 1 Pattern propagates outward, forming a cone of recurrent hotspots
- 2 Pattern does not really depend on the initial condition

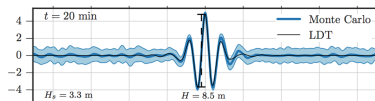


Coherent structures: how does the bump look up close?

A new class of localized solutions depending on the background P



[A., Athanassoulis, Sapsis, JOEME (2017)]
via scaling of unstable modes

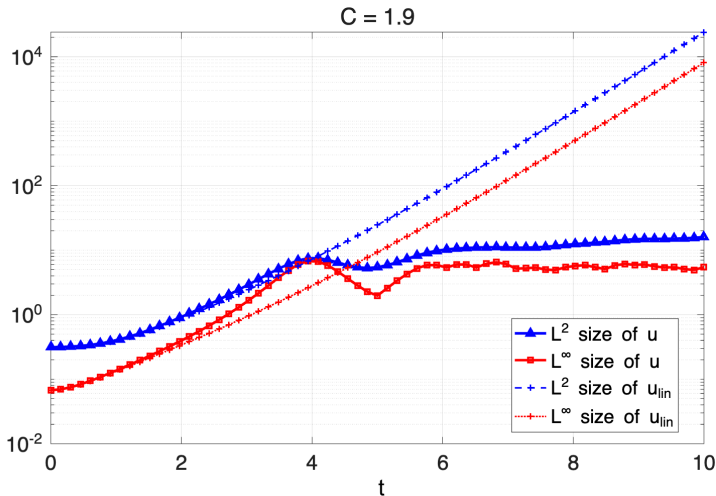


[Dematteis, Grafke, Vanden-Eijden, PNAS (2018)]

Monte Carlo + Large Deviations Theory
for fully Nonlinear simulations of mNLS

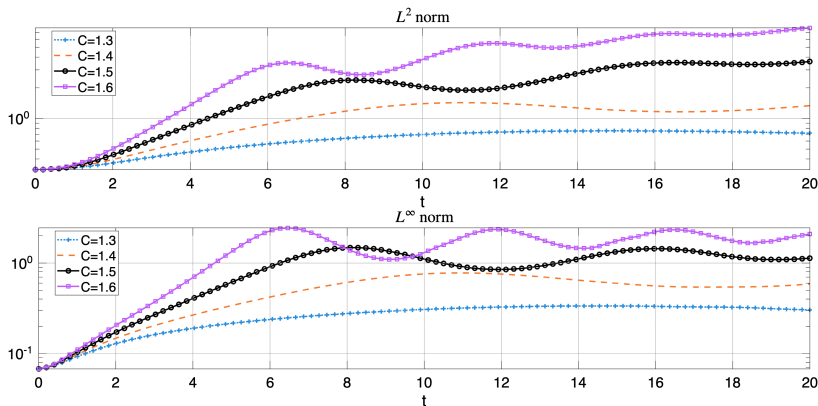
Linear vs. nonlinear: rate of growth

- 1 Linear theory predicts the initial rate of growth
- 2 Nonlinear effect: saturation (coherent structures)



Phenomenology of the bifurcation

Main finding: values saturate at lower level as $C \rightarrow C_*^+$



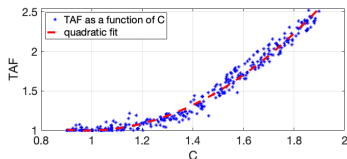
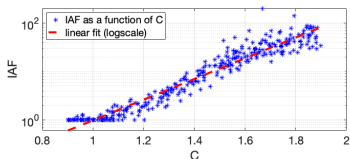
Monte Carlo for localized extremes

C drawn uniformly from $[0.9, 1.9]$; random initial perturbations.

Two measures of amplification, inspired by

[Stiassnie, Regev & Agnon, J. Fluid Mech. 2008; Ribal, Babanin, Young, Toffoli & Stiassnie, J. Fluid Mech. 2013]

- **IAF** (Inhomogeneity Amplification Factor): $\frac{\max_{t,x,y} |u|}{\max_{x,y} |u_0|}$
- **TAF** (Total Amplification Factor): $\frac{\max_{t,x,y} |u + \Gamma|}{\Gamma(0)}$



Key findings: amplification depends primarily on the background intensity, not on the specific initial perturbation. Borderline unstable problems very muted.

Summary and outlook

The numerical method:

- Relaxation-CN scheme for the Alber/von Neumann equation: linearly implicit, $O(\tau^2 + h^4)$, structure-preserving
- Advanced initialization recovers full $O(\tau^2)$ accuracy in time
- Full stability/convergence analysis requires Schatten class norms
open problem \mapsto [arXiv:2604.16998](https://arxiv.org/abs/2604.16998) for related advances in theory

Onset of modulation instability:

- Linear theory captures initial growth rate, misses saturation level
- IAF and TAF depend on the background, not on the perturbation
- Space-time lattice of hotspots in the nonlinear regime
- Recurrent hotspots a possible mechanism for rogue waves

Thank you!