Evolution of quantum knots driven by minimal surfaces

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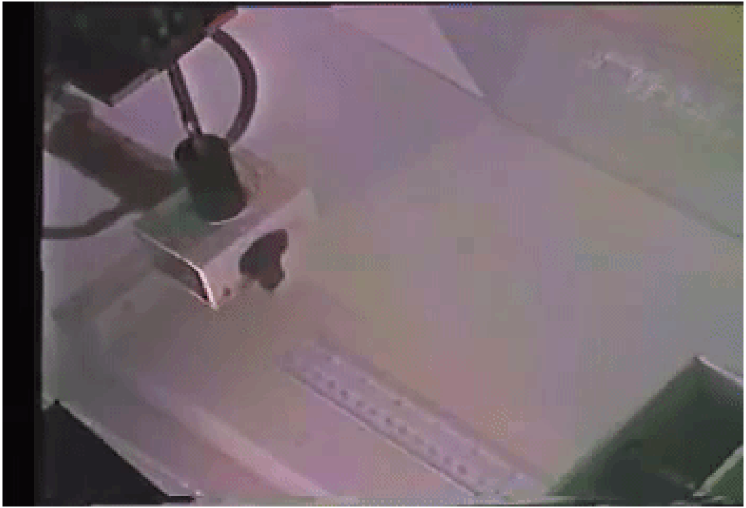
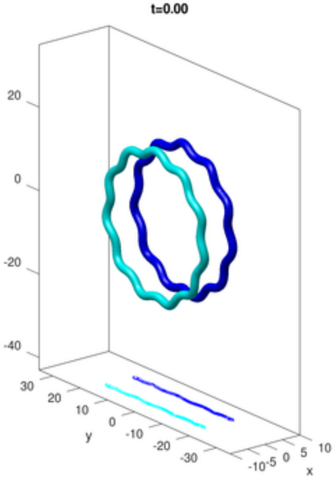
September 3rd, 2022

Fundamental changes in the topology, Lim & Nickels (1992)



Head-on collision of perturbed quantum vortex rings under the GPE



Agenda

Agenda

The Gross-Pitaevskii equation (GPE)

For a **weakly interacting Bose-Einstein condensate**,

$$\psi_t = \frac{\mathrm{i}}{2}\nabla^2\psi + \frac{\mathrm{i}}{2}(1 - |\psi|^2)\psi. \qquad (1)$$

By introducing the **Madelung transformation** $\psi = \sqrt{\rho}e^{\mathrm{i}\theta}$, from which $\rho = |\psi|^2$ **and** $\mathbf{u} = \nabla\theta$, GPE can be recast in the form of the **Navier-Stokes equations**. However, vortex defects are **strictly localized** and no threads or bridges of weaker vorticity are visible, contrary to viscous flows.

$\Rightarrow$ **Numerical problem**. For dark structures $\rho \to 1$ as $|\mathbf{x}| \to \infty$ and a spectral approach based on FFT needs a **periodic initial solution on a truncated domain**. If $\psi_0(\boldsymbol{x})$ is not periodic, it **must be mirrored** with consequent higher computational effort and larger memory requirements. Because of limited computational resources, the **numerical box might be too small**.

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The Free-Boundary Time-Splitting Finite-Difference method

$\Rightarrow$ **Solution** proposed by Caliari & Zuccher (2021).

- We perform a **change of variable** $\eta(\boldsymbol{y}, t) = \psi(\boldsymbol{x}, t)$, to map $\boldsymbol{x} \in \mathbb{R}^3$ into $\boldsymbol{y} \in (-1, 1)^3$ and choose $y_\ell(x_\ell) = \frac{2}{\pi} \arctan\left(\frac{x_\ell}{\alpha_\ell}\right), \alpha_\ell > 0$
- We discretize in space with **4th-order finite differences**, near the boundaries we use one-sided 4th-order finite differences, obtaining the GPE in the form

$$z'(t) = Az(t) + \frac{\mathrm{i}}{2}\left(1 - |z(t)|^2\right) z(t), \tag{2}$$

  where $z(t)$ is a vector of dimension (degree of freedom) $M = m_1 \times m_2 \times m_3$.
- We apply the **Strang time splitting** to the system above, thus yielding a new method that we call **Free Boundary Time Splitting Finite Difference (FBTSFD)** method. We solve the linear part of (2) by an **efficient approximation of the action of the matrix exponential** at machine precision accuracy; the nonlinear part is solved exactly.

Generation of the initial condition for the GPE

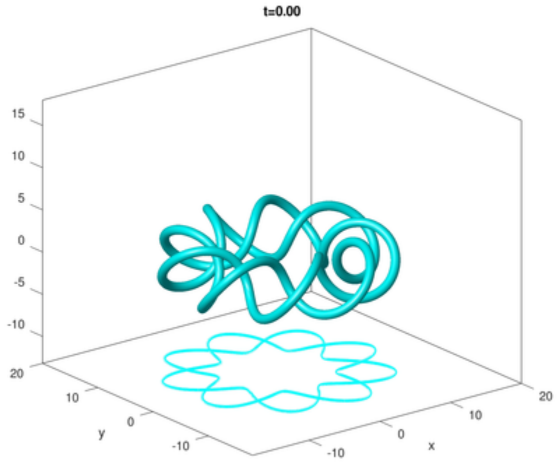
We know how to deal with a single **straight vortex** (see Caliari and Zucher (2018)) and a single **vortex ring** (see Zuccher and Caliari (2021)).

For an **arbitrary initial condition** this is what we did.

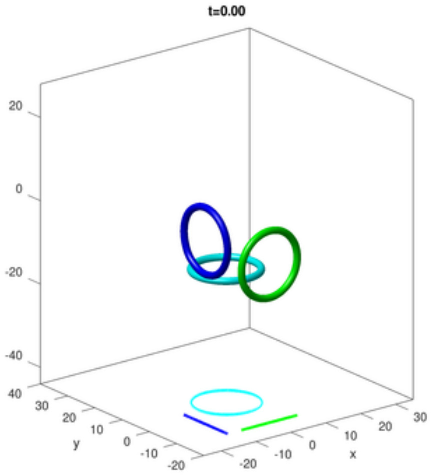
- **Biot–Savart** integral to compute the velocity field $\boldsymbol{u}(\boldsymbol{x})$ at each position $\boldsymbol{x}$.
- **Integrate** the equation $\boldsymbol{u} = \nabla\theta$ **to get the phase** $\theta(\boldsymbol{x})$, after setting a reference value θ_0 at a certain point $\boldsymbol{x}_0 \in \Omega$.
- To **avoid vortex-line singularities**: we set $\theta = 0$ at a point sufficiently distant from a defect line and integrate along paths that start from that point and go either towards infinity or terminate on the defect line.
- Assign **density** $\rho(\boldsymbol{x})$ **according to the 4th-order Padé approximation** of the steady straight vortex. Since $\rho = \rho(r)$, for each grid point choose r as the minimum distance from the closest vortex centerlines.

Agenda

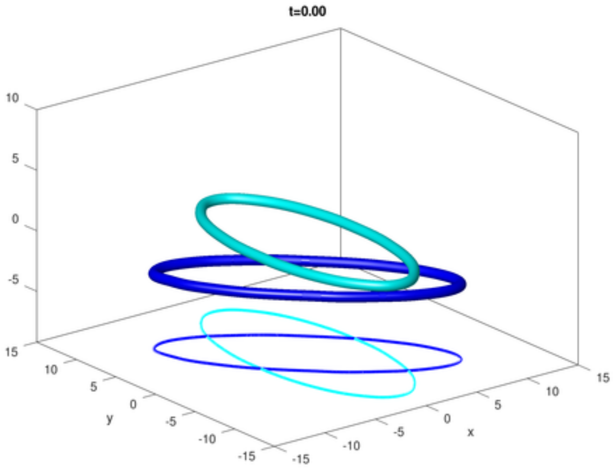
Time evolution and topological cascade of the torus knot $\mathcal{T}(2,9)$



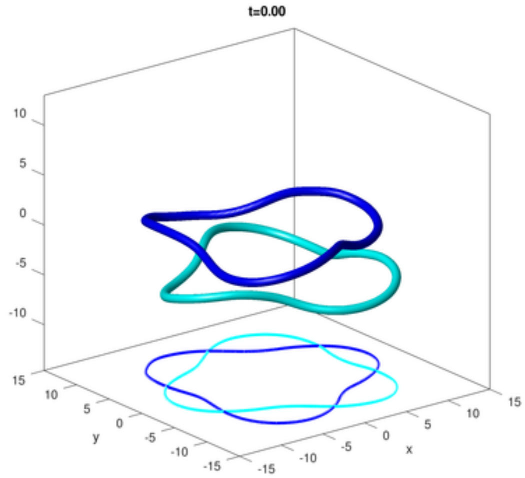
Collision of three unlinked and mutually orthogonal rings



Hopf link generated by two unlinked, unknotted elliptical defects

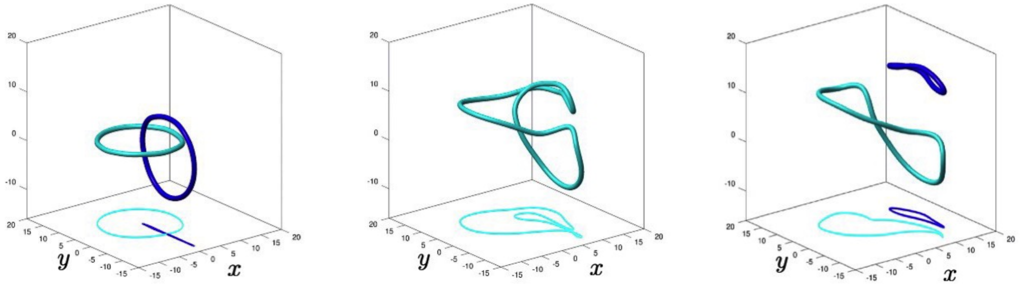


Generation of a trefoil knot from two unlinked, perturbed rings



Agenda

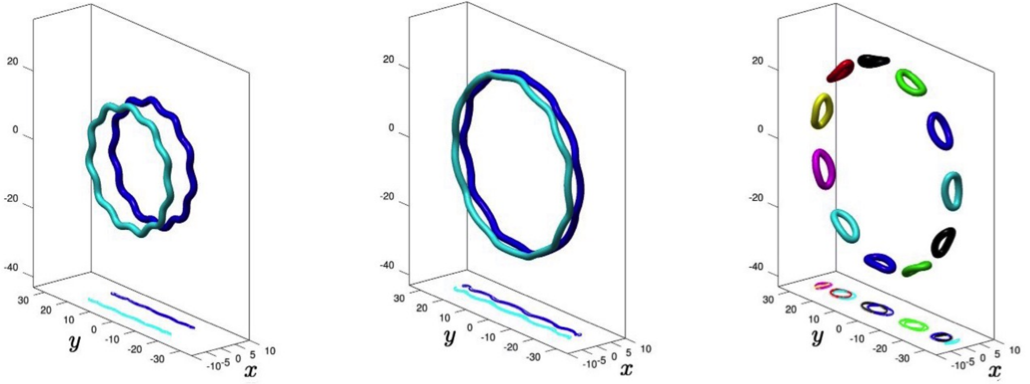
1. Direct topological *cascade* and collapse: Hopf link $\mathcal{T}(2,2)$



$t = 8.80$ $t = 39.20$ $t = 49.60$

Evolution of Hopf link $\mathcal{T}(2,2)$: first reconnection to form a single unlinked, unknotted loop $\mathcal{T}(2,1)$ that reconnects again to form two separate small loops $\mathcal{T}(2,0)$.

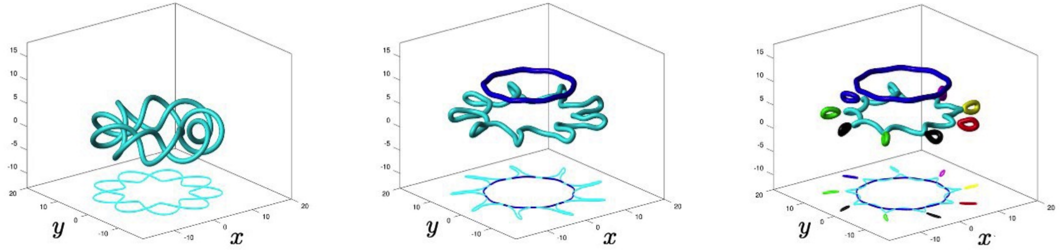
1. Direct topological cascade and *collapse*: HOC of perturbed rings



$t = 0.00$ $t = 42.80$ $t = 56.00$

As two perturbed vortex rings approach each other they stretch; when they are close the symmetric perturbations give rise to 11 simultaneous reconnections, equi-spaced all along the reconnection circular region; 11 small vortex rings are generated, propagating radially away from the reconnection region

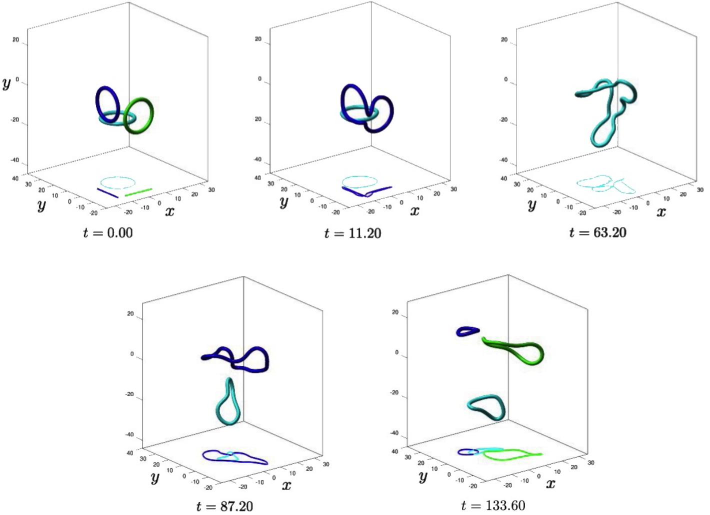
1. Direct topological cascade and *collapse*: torus knot $\mathcal{T}(2,9)$



$t = 0.00$ $t = 30.40$ $t = 32.80$

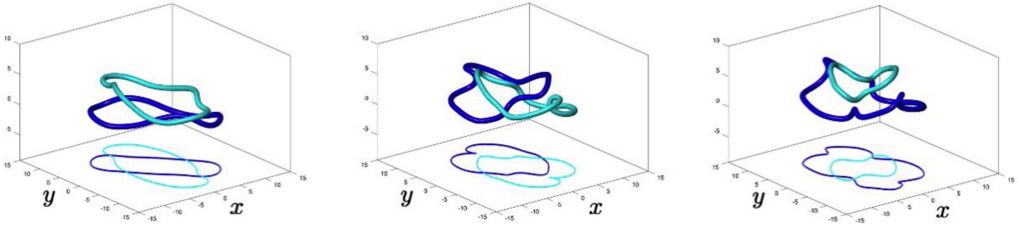
Evolution of $\mathcal{T}(2,9)$: by symmetry the 9 helical coils of the knot produce 9 simultaneous reconnections. The knot type $\mathcal{T}(2,9)$ jumps directly to $\mathcal{T}(2,0)$ creating 2 separate loops: the leading ring (dark blue) and a convoluted trailing loop behind. The latter undergoes 9 simultaneous reconnections creating 9 small vortex rings. In this case the cascade process is realized by the topological collapse of a large, single structure to produce first a medium-sized , and then small-scale structures.

2. *Structural* and topological cycles: 3 mutually orthogonal rings



Structural cycle: 3 loops → 2 loops → 1 loop → 2 loops → 3 loops.

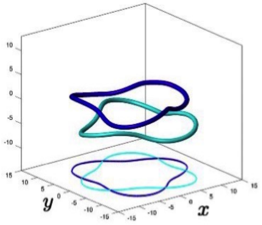
2. Structural and *topological* cycles: creation of Hopf link



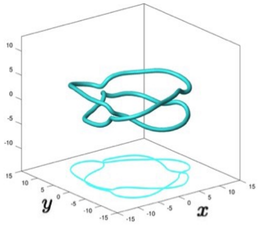
$t = 6.40$ $t = 11.60$ $t = 15.20$

Topological cycle, generation of Hopf link with a temporary increase of topology from 2 planar ellipses: 2 unlinked loops $\rightarrow$ Hopf link $\mathcal{T}(2,2)$ $\rightarrow$ 2 unlinked loops.

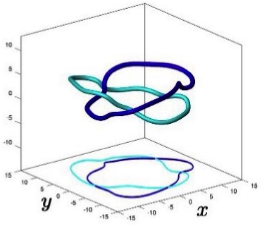
3. Inverse topological cascade: creation of trefoil knot



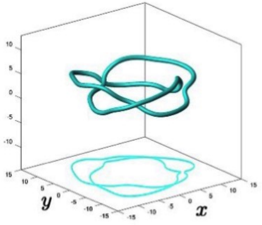
$t = 0.00$



$t = 8.80$



$t = 13.60$



$t = 17.60$

Inverse topological cascade: **evolution of topologically simple structures to produce more complex ones**. 2 initially disjoint, unknotted and unlinked perturbed rings interact to create first a single convoluted loop, then a Hopf link, and finally a trefoil knot. **First realization** of a topologically non-trivial knot starting from topologically trivial initial conditions (unlinked, unknotted loops).

2 loops $\mathcal{T}(2,0)$ → 1 loop $\mathcal{T}(2,1)$ → Hopf link $\mathcal{T}(2,2)$ → trefoil knot $\mathcal{T}(2,3)$

Agenda

Topological quantum hydrodynamics

Quantized circulation $\Gamma = 2\pi n$, $n \in \mathbb{N}$. **Kinetic helicity** $\mathcal{H} = \int_\Omega \mathbf{u} \cdot \omega \, dV$ where $\omega = \nabla \times \mathbf{u}$ and $V = V(\Omega)$ is the volume of the vorticity region Ω.
In quantum systems vorticity is singular on $\mathcal{C}$ and the domain of vorticity has measure zero (in distributional sense) thus

$$\mathcal{H} = \Gamma \oint_{\mathcal{C}} \mathbf{u} \cdot d\mathbf{X} = \Gamma \oint_{\mathcal{C}} \nabla\theta \cdot d\mathbf{X} = 0, \qquad \text{zero-helicity condition.} \tag{3}$$

If vorticity is localized on N thin filaments $\mathcal{C}_i$ $(i = 1, \ldots, N)$

$$\mathcal{H} = \sum_i \Gamma_i Sl_i + \sum_{i \neq j} \Gamma_i \Gamma_j Lk_{ij}\,, \qquad Sl_i = Wr_i + Tw_i, \tag{4}$$

where Sl_i is the **Călugăreanu self-linking number** (topological invariant of the i-th defect), and Lk_{ij} is the **Gauss linking number** (topological invariant of the link between defects i and j, with $i \neq j$, $i, j = 1, \ldots, N$).
Wr_i is the **writhing number** and Tw_i is the **total twist**.

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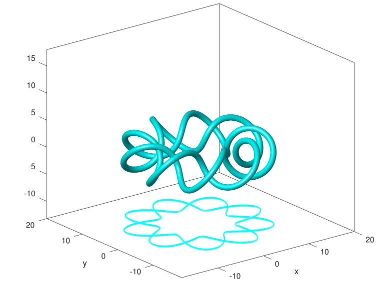
T29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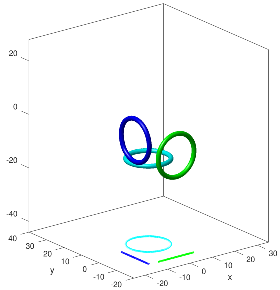
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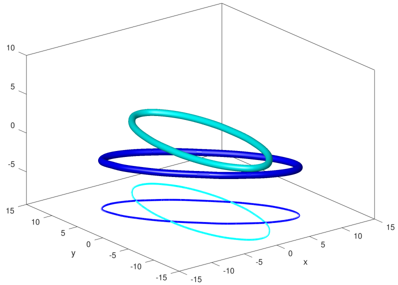
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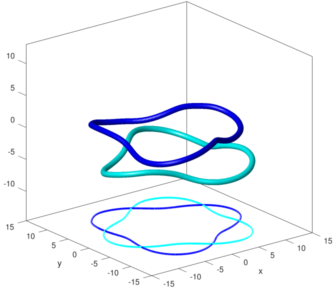
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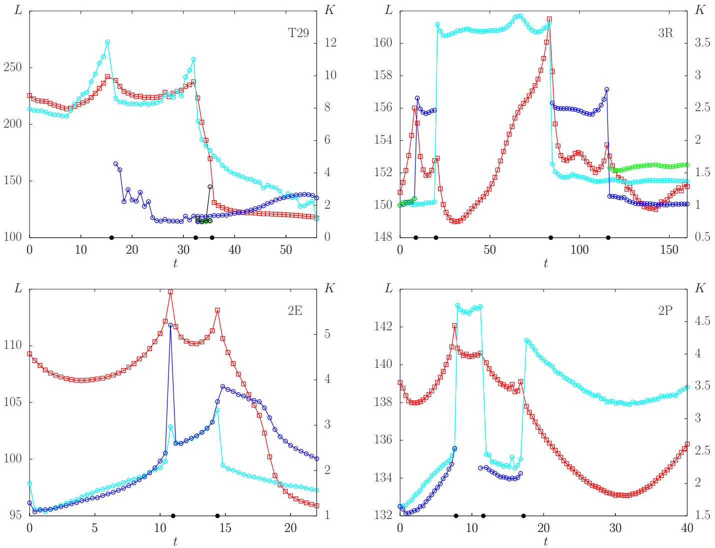
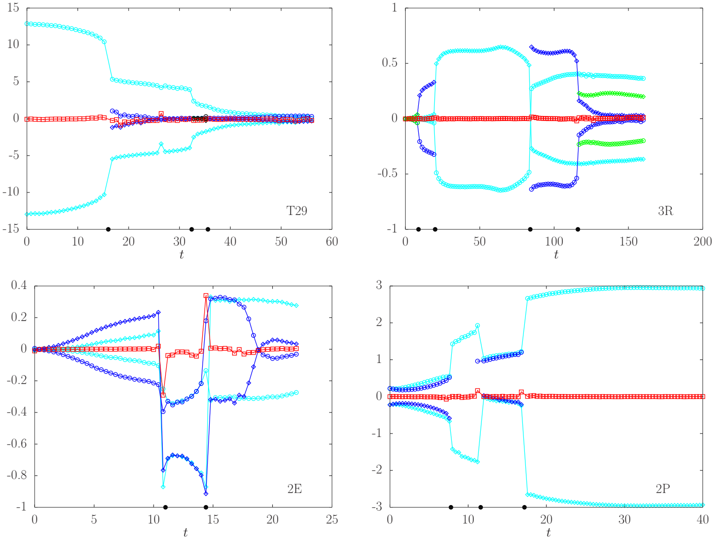
Total length L (red squares) and normalized total curvature K



L increases as defects get closer; the **rate of change** $|\delta L/\delta t|$ is larger after reconnections due to higher curvature of the recombined strands right after reconnection (time asymmetry and irreversibility due to **sound emission**). Pronounced **picks and drops of K** mark accurately the occurrence of **reconnection events**.

Writhe *Wr* ○, total twist *Tw* ◇ and helicity $\mathcal{H}$ □ (red)



$\mathcal{H} \equiv 0$, total twist conserved across reconnections. Apparently unbalanced jumps in 2E and 2P due to generation of Hopf link, i.e $|\Delta Lk_{12}| = 1$. **Direct topological cascade** or collapse (T29): decrease in writhe, progressive decay towards unlinked, unknotted planar rings. Behavior partially reversed under **cyclic phenomena** (3R and 2E), completely reversed for **inverse cascade** (2P).

Agenda

GPE – energy contributions

The non-dimensional form of total energy $E_{\rm tot}$, **constant under GPE**, is given by

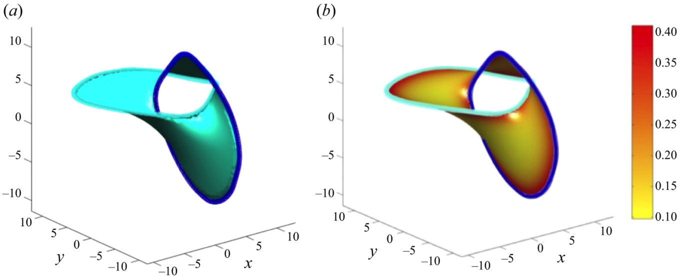
$$E_{\rm tot} = \int \left(\frac{1}{2}|\nabla\psi|^2 - \frac{1}{2}|\psi|^2 + \frac{1}{4}|\psi|^4 \right) dV \, . \tag{5}$$

By Madelung's transformation $|\nabla\psi|^2 = \rho|\nabla\theta|^2 + \dfrac{|\nabla\rho|^2}{4\rho} = \rho|\mathbf{u}|^2 + \dfrac{|\nabla\rho|^2}{4\rho}$, hence

$$E_{\rm tot} = \underbrace{\frac{1}{2}\int \rho|\mathbf{u}|^2 \, dV}_{E_k} + \underbrace{\frac{1}{8}\int \frac{|\nabla\rho|^2}{\rho} \, dV}_{E_q} - \underbrace{\frac{1}{2}\int \rho \, dV}_{E_p} + \underbrace{\frac{1}{4}\int \rho^2 \, dV}_{E_i} \, . \tag{6}$$

Density ρ reaches a constant value outside the healing region $O(\xi)$, but decays rapidly to zero inside the healing region, thus E_p **and** E_i can be taken to be constant everywhere **outside the healing regions** and **ignored**.

Minimal surface as critical energy surface



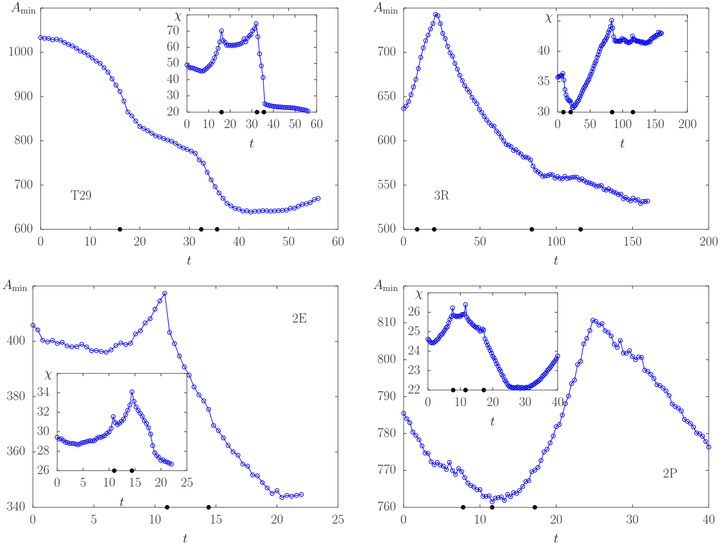
(a) Isophase surface $S_{\rm min}$; (b) same surface color-coded by the sum $e_{\rm k} + e_{\rm q}$

Let $S'_{\rm min}$ be the portion of the minimal isophase surface $S_{\rm min}$ where **density is almost constant** and compressibility is negligible. $A(S'_{\rm min}) \approx A(S_{\rm min}) = A_{\rm min}$ because excluded area is small. Since $\mathbf{u} = \nabla\theta$, where $\rho \approx$ constant $\nabla\cdot\mathbf{u} = 0 \Rightarrow \nabla^2\theta = 0\ \forall\mathbf{x}\in S'_{\rm min}$.

This shows that $S'_{\rm min}$ is **harmonic** and, being a conformal immersion in $\mathbb{R}^3$, it is critical with respect to the **Dirichlet functional** $D(\Theta) = \frac{1}{2}\int_{S'_{\rm min}}|\nabla\Theta|^2 dS$. **Minimal isophase surfaces** are thus **privileged markers** for energy because

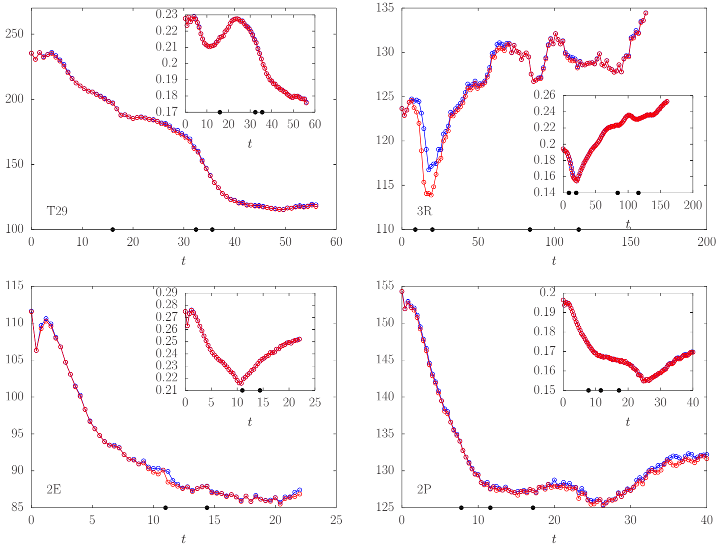
$$D(\psi)|_{S_{\rm min}} = \frac{1}{2}\int_{S_{\rm min}}|\nabla\psi|^2 dS = \frac{1}{2}\int_{S_{\rm min}}\left[\rho|\mathbf{u}|^2 + \frac{|\nabla\rho|^2}{4\rho}\right]dS = \int_{S_{\rm min}}(\mathbf{e}_{\rm k}+\mathbf{e}_{\rm q})dS = \mathcal{E}_{\rm k}+\mathcal{E}_{\rm q}\ .$$

$A_{\min} = A(S_{\min})$ of isophase surface; insets show $\chi = L^2/A_{\min}$



Direct topological cascade T29: monotonic decrease of $A_{\min}$, which increases after the formation of small rings. **Structural cycle** 3R: $A_{\min}$ is maximum when a single loop is present then monotonically decreases towards small rings. **Topological cycle** 2E: same behavior. **Inverse cascate** 2P: increase of $A_{\min}$, peak at $t \approx 27$, then decrease of $A_{\min}$. Evolutionary decay processes are indeed **minimal surface energy relaxation processes**.

$\mathrm{Max}[D(\psi)]$ (blue) for $\theta \in [0, 2\pi)$, and of $D(\psi)|_{S_{\mathrm{min}}}$ (red)



Plots **coincide almost everywhere** for all the cases, confirming that S_{min} is indeed critical for energy, and proves to be an **appropriate marker for dynamics**.

Plots in **insets** show the **average values** given by $\mathrm{Max}[\overline{\mathcal{E}}_{\mathrm{kq}}(S)]$ (blue) and $\overline{\mathcal{E}}_{\mathrm{kq}}|_{S_{\mathrm{min}}}$ (red): **correlation** between **minimal surface energy relaxation** and direct topological cascade is quite evident.

Agenda

Conclusions

1. Direct numerical simulations of the GPE based on a new approach that **resolves the limits** imposed by boundary conditions on a **truncated domain**.
2. Several test cases analyzed, **3 possible scenarios**: direct cascade and collapse, structural and topological cycles and inverse cascade.
3. Generation, for the first time ever, of a **trefoil knot** from the interaction of two unlinked, unknotted loops.
4. **Time asymmetry** of reconnections due to sound emission **confirmed** by length rate of change, see also total curvature.
5. **Zero Helicity Theorem confirmed**: balance between writhe, twist and linking number. Gradual nullification of writhe in decaying processes.
6. **Defect dynamics driven by $S_{\rm min}$**, $\mathrm{Max}[D(\psi)]$ corresponds to $D(\psi)|_{S_{\rm min}}$.
7. Direct topological cascade detected by a **monotonic decrease of $A_{\rm min}$**, consistent with the observed **energy relaxation**.

Some references

- Zuccher, S. & Ricca, R. L. 2022, Creation of quantum knots and links driven by minimal surfaces, *Journal of Fluid Mechanics*, **942**, A8.
- Caliari, M. & Zuccher, S. 2021, A fast Time Splitting Finite Difference approach to Gross-Pitaevskii equations, *Communications in Computational Physics*, **29**, 1336-1364.
- Zuccher, S. & Caliari, M. 2021, Accurate numerical determination of a self-preserving quantum vortex ring, *Journal of Physics A: Mathematical and Theoretical*, **54**, 015301.
- Caliari, M. & Zuccher, S. 2018, Reliability of the time splitting Fourier method for singular solutions in quantum fluids, *Computer Physics Communications*, **222**, 46-58.

Questions?

$\mathcal{H} = \sum_i \Gamma_i \left(Wr_i + Tw_i \right) + \sum_{i \neq j} \Gamma_i \Gamma_j Lk_{ij} = 0$

Writing number $Wr_i = Wr(\mathcal{C}_i)$ is a global geometric property of a space curve $\mathcal{C}_i$

$$Wr_i = \frac{1}{4\pi} \oint_{\mathcal{C}_i} \oint_{\mathcal{C}_i} \frac{(\mathbf{X}_i - \mathbf{X}_i^*) \cdot d\mathbf{X}_i \times d\mathbf{X}_i^*}{|\mathbf{X}_i - \mathbf{X}_i^*|^3}, \qquad Wr_i \in \mathbb{R}, \tag{7}$$

where $\mathbf{X}_i$ and $\mathbf{X}_i^*$ denote two distinct points on $\mathcal{C}_i$.

Total twist number $Tw_i = Tw(\mathcal{R}_i)$ is a global geometric property of a space curve $\mathcal{C}_i$: given the ribbon $\mathcal{R}_i$ identified by the unit vector $\hat{\mathbf{U}} = \hat{\mathbf{U}}(s)$, on $\mathcal{C}_i$

$$Tw_i = \frac{1}{2\pi} \oint_{\mathcal{C}_i} \left(\hat{\mathbf{U}} \times \frac{d\hat{\mathbf{U}}}{ds} \right) \cdot \hat{\mathbf{T}}\, ds \qquad Tw_i \in \mathbb{R}. \tag{8}$$

Twist is independent of the particular Seifert (isophase) surface chosen.

Linking number $Lk_{ij} = Lk(\mathcal{C}_i, \mathcal{C}_j)$ is a topological invariant between defects i and j

$$Lk_{ij} = \frac{1}{4\pi} \oint_{\mathcal{C}_i} \oint_{\mathcal{C}_j} \frac{(\mathbf{X}_i - \mathbf{X}_j) \cdot d\mathbf{X}_i \times d\mathbf{X}_j}{|\mathbf{X}_i - \mathbf{X}_j|^3}, \qquad Lk_{ij} \in \mathbb{Z}, \tag{9}$$

where $\mathbf{X}_i \in \mathcal{C}_i$ and $\mathbf{X}_j \in \mathcal{C}_j$. Note that $Wr_i = Lk_{ii}$.

Details on initial conditions (1/2)

Perturbed rings have centerlines

$$\mathbf{X} : \begin{cases} X(t) = \left[R + A_{\mathrm{i}} \cos(mt)\right] \cos t \ , \\ Y(t) = \left[R + A_{\mathrm{i}} \cos(mt)\right] \sin t \ , \\ Z(t) = A_{\mathrm{o}} \cos\left[m(t - \frac{\pi}{6})\right] \ , \end{cases} \tag{10}$$

where R is the radius of the unperturbed ring, A_{i} the perturbation of the components in the xy-plane, A_{o} the perturbation of the out-of-plane component, and m the wavenumber.

Torus knots $\mathcal{T}(p, q)$ are given by

$$\mathbf{X} : \begin{cases} X(t) = \left[R + r\cos(qt)\right] \cos(pt) \ , \\ Y(t) = \left[R + r\cos(qt)\right] \sin(pt) \ , \\ Z(t) = r\sin(qt) \ , \end{cases} \tag{11}$$

where R and r are respectively the large and small radius of the torus $\mathbb{T}$, p and q the number of wraps along the longitudinal and meridian (poloidal) direction of $\mathbb{T}$.

Details on initial conditions (2/2)

HOC: 2 rings of radius $R = 17.4$ perturbed according to eqs. (10), with $A_\mathrm{i} = 0.8$, $A_\mathrm{o} = 0.22$ and wavenumber $m = 11$, are placed in two parallel planes $x = \pm 4$ mirror-imaging one another.
T29: knot $\mathcal{T}(2, 9)$ given by eqs. (11), with $R = 10$, $r = 3.3$, $p = 2$ and $q = 9$, placed at the origin.
3R: 3 self-preserving rings with radius $R = 8$; first ring centered at $(-12, -4, 0)$ moving in the positive direction of x_1 ($\equiv x$), second ring centered at $(0, -12, -6)$ moving in the positive direction of x_2 ($\equiv y$), third ring centered at $(0.5, 4.5, -12)$ moving in the positive direction of x_3 ($\equiv z$).
2E: 2 ellipses given in parametric form by $(a \cos t, b \sin t)$; first ellipse of semi-axes $a = 5$ and $b = 12$ centered at the origin; second ellipse of semi-axes $a = 4$ and $b = 12$ centered at $(0, 0, -3)$ and rotated by $\pi/4$ with respect to the first.
2P: 2 rings of radius $R = 10$, perturbed according to eqs. (10) with $A_\mathrm{i} = 2$, $A_\mathrm{o} = 1$ and wavenumber $m = 3$; first ring centered at the origin, second ring centered at $(1, 0, -4)$ and rotated by $\pi/3$ with respect to the first.

Further numerical details

Case	$N_x \times N_y \times N_z$	$\alpha_1, \alpha_2, \alpha_3$	Physical domain	Δt	IC
HOPF	$171 \times 171 \times 171$	$15, 15, 15$	$[-821, 821]^3$	0.02	ZR
HOC	$187 \times 187 \times 187$	$15, 15, 15$	$[-898, 898]^3$	0.02	BS
T29	$171 \times 171 \times 171$	$15, 15, 15$	$[-821, 821]^3$	0.02	BS
3R	$171 \times 171 \times 171$	$15, 15, 15$	$[-821, 821]^3$	0.02	SP
2E	$171 \times 171 \times 171$	$15, 15, 15$	$[-821, 821]^3$	0.02	BS
2P	$171 \times 171 \times 171$	$15, 15, 15$	$[-821, 821]^3$	0.02	BS

Table: Case considered, degrees of freedom $N_x \times N_y \times N_z$, α_k-values ($k = 1, 2, 3$), physical domain, time-step Δt and type of initial condition: ZR, rings generated as in ZR17; BS, Biot-Savart generation; SP, self-preserving rings generated by the product of initial conditions $\psi_{0\nu}$ ($\nu = 1, 2, 3$) for each of the 3 self-preserving rings.