Numerical simulation of the Gross–Pitaevskii equation *via* vortex-tracking

Gaspard Kemlin
https://gaspardkemlin.frama.io/

LAMFA, Université de Picardie Jules Verne – CNRS UMR 7352

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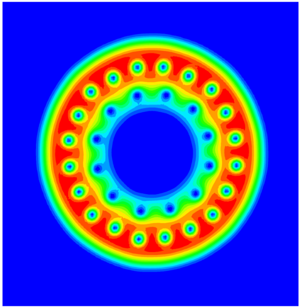
Vortices in the Gross–Pitaevskii equation

Model for rotating Bose–Einstein condensates[1]

$$\imath\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi + g|\psi|^2\psi + \imath\hbar\Omega A^t\nabla\psi \quad \text{where } A^t = (y, -x, 0).$$

$\rightsquigarrow$ vortices are isolated zero of the wave function with nonzero winding number (degree): typical form for ψ around a vortex is $f(r)e^{\imath\theta}$ with $f(0) = 0$ and $f(r_0) = 1$.

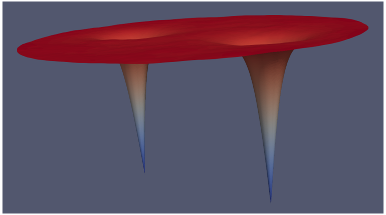


[1] V. Kalt, G. Sadaka, I. Danaila, and F. Hecht. Identification of vortices in quantum fluids: Finite element algorithm and programs. *Computer Physics Communications*, 284:108606, 2023.

A toy model is given by the Ginzburg–Landau energy functional:

$$E_\varepsilon(u) = \int_\Omega |\nabla u|^2 + \frac{1}{4\varepsilon^2}(1-|u|^2)^2,$$

where $\Omega \subset \mathbb{R}^2$ is smooth, bounded and simply connected. $\varepsilon > 0$ is a small parameter, linked to the size of vortices.



Given $g : \partial\Omega \to \mathbb{S}^1 \subset \mathbb{C} \simeq \mathbb{R}^2$, we consider the minimization problem

$$u_\varepsilon \in \operatorname{argmin}\left\{E_\varepsilon(u),\ u \in H^1(\Omega,\mathbb{C}),\ u = g \text{ on } \partial\Omega\right\} \Rightarrow \begin{cases} -\Delta u_\varepsilon = \dfrac{1}{\varepsilon^2}(1-|u_\varepsilon^2|)u_\varepsilon & \text{in } \Omega, \\ u = g & \text{on } \partial\Omega. \end{cases}$$

We study the minimizers when $\varepsilon \to 0$ and $\deg(g,\partial\Omega) \neq 0$ (the winding number of $g : \partial\Omega \to \mathbb{S}^1 \approx$ the number of times it goes around zero).

Morally: when $\varepsilon \to 0$, $|u_\varepsilon| \to 1$ but then $\displaystyle\int_\Omega |\nabla u_\varepsilon|^2 \to +\infty$ (otherwise, we can find a limit $\widetilde{u}$ s.t. $u_\varepsilon \to \widetilde{u}$ a.e., with $\widetilde{u} \in H^1(\Omega,\mathbb{S}^1)$ and $\deg(\widetilde{u},\partial\Omega) = \deg(g,\partial\Omega) \neq 0 \Rightarrow$ topologically impossible).

Theorem (The canonical harmonic map[2])

There exists $u^*(\cdot; \boldsymbol{a})$ and $d = deg(g, \partial\Omega) \neq 0$ points $\boldsymbol{a} = (a_1, \dots, a_d)$ in Ω such that $u_\varepsilon \to u^*(\cdot; \boldsymbol{a})$ (up to extraction).

- The map $u^*(\cdot, \boldsymbol{a}) : \Omega \to \mathbb{S}^1$ is called the canonical harmonic map associated to the points $\boldsymbol{a} = (a_1, \dots, a_d)$ and there exists a harmonic function $H : \mathbb{R}^2 \simeq \mathbb{C} \to \mathbb{R}$ such that

$$\boxed{u^*(x; \boldsymbol{a}) = \mathrm{e}^{\imath H(x)} \prod_{j=1}^{d} \frac{x - a_j}{|x - a_j|}.}$$

- H is defined such that u^* satisfies the boundary conditions.

[2] F. Bethuel, H. Brezis, and F. Hélein. Ginzburg-Landau Vortices. *Birkhäuser Boston*, 1994.

Theorem (The renormalized energy[3])

The vortices coordinates $\boldsymbol{a} = (a_j)_{1 \leqslant j \leqslant d}$ is a minimizer of the renormalized energy W on Ω^d.

- The renormalized energy W is defined, for $\boldsymbol{b} = (b_1, \ldots, b_d)$, by

$$W(\boldsymbol{b}) = \underbrace{-\pi \sum_{i \neq j} \ln |b_i - b_j|}_{\text{Interaction term}} + \underbrace{W_{\mathrm{bc}}(\boldsymbol{b})}_{\text{Boundary term}} \approx \lim_{\varepsilon \to 0} E_\varepsilon(u_\varepsilon) - d\left(\pi \underbrace{\ln(1/\varepsilon)}_{\text{Self-energy}} + \underbrace{\gamma}_{\text{Universal constant}}\right).$$

- $W \to +\infty$ as two points coalesce (interaction term) or when one point gets close to $\partial\Omega$ (boundary term).

[3] F. Bethuel, H. Brezis, and F. Hélein. Ginzburg-Landau Vortices. *Birkhäuser Boston*, 1994.

Time-dependent case

We now consider the following time-dependent Gross–Pitaevskii equation, obtained from the Schrödinger flow $\imath\partial_t\psi_\varepsilon = -\nabla E_\varepsilon(\psi_\varepsilon)$ of the Ginzburg–Landau energy functional, with Neumann boundary conditions:

(GPE)
$$\begin{cases} \imath\dfrac{\partial\psi_\varepsilon}{\partial t} = \Delta\psi_\varepsilon + \dfrac{1}{\varepsilon^2}(1-|\psi_\varepsilon|^2)\psi_\varepsilon \text{ in } \Omega, \\ \partial_\nu\psi_\varepsilon(\cdot,t) = 0 \text{ on } \partial\Omega \quad \text{and} \quad \psi_\varepsilon(\cdot,0) = \psi_\varepsilon^0. \end{cases}$$

- We are not interested in minimizers anymore: we rather study the evolution of an initial wave function ψ_ε^0 which is made of "almost vortices".
- Vorticity not restricted anymore to $d_j = +1$: $d_j = -1$ is now allowed too.

Assuming that

- the *vorticity* of ψ_ε^0 converges, when $\varepsilon \to 0$, to a sum of Dirac masses with given locations $\boldsymbol{a}^0 \in \Omega^N$ and degrees $d \in \{\pm 1\}^N$:

$$J\psi_\varepsilon^0 \to \pi \sum_{j=1}^N d_j \delta_{a_j^0}, \quad \text{with} \quad J\psi = \frac{1}{2}\nabla \times j(\psi) \text{ and } j(\psi) = \frac{1}{2\imath}(\overline{\psi}\nabla\psi - \psi\nabla\overline{\psi}) = \text{super-current};$$

- the initial energies $E_\varepsilon(\psi_\varepsilon^0)$ are bounded by: $E_\varepsilon(\psi_\varepsilon) \leq \pi N \ln(1/\varepsilon) + C$.

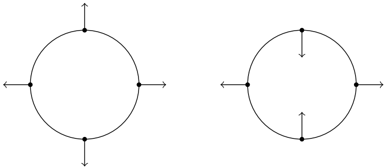
Then, for $t > 0$, $J\psi_\varepsilon(t) \to \pi \sum_{j=1}^N d_j \delta_{a_j(t)}$, where $\boldsymbol{a}(t)$ solves, with $\mathbb{J} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$,

$$\text{(HD)} \quad \begin{cases} \dot{a}_j(t) = -\frac{1}{\pi} d_j \mathbb{J} \nabla_{a_j} W(\boldsymbol{a}(t), d), \\ a_j(0) = a_j^0, \end{cases} \quad \text{where } W(\boldsymbol{a}, d) = -\pi \sum_{1 \leq i \neq j \leq N} d_i d_j \ln|a_i - a_j| + W_{\text{bc}}(\boldsymbol{a}, d).$$

[4] J. Colliander and R. Jerrard. Vortex dynamics for the Ginzburg-Landau-Schrodinger equation. *International Mathematics Research Notices*, 1998(7):333, 1998.

[5] F.-H. Lin and J. X. Xin. On the Incompressible Fluid Limit and the Vortex Motion Law of the Nonlinear Schrödinger Equation. *Communications in Mathematical Physics*, 200(2):249–274, 1999.

Convergence results



Results also characterize

- $\psi_\varepsilon(t) \to u^*(\cdot; \boldsymbol{a}(t), d)$ in $W^{1,p}(\Omega)$, $p < 2$,
- $j(\psi_\varepsilon(t)) \to j(u^*(\cdot; \boldsymbol{a}(t), d))$ in $L^p(\Omega)$, $p < 2$,

Here, $u^*(\cdot; \boldsymbol{a}, d)$ with values in $\mathbb{S}^1$ is the uniquely determined harmonic map with singularities at locations $\boldsymbol{a}$ with local degrees d, and with boundary conditions:

$$u^*(x; \boldsymbol{a}, d) = e^{\imath H(x)} \prod_{j=1}^{N} \left(\frac{x - a_j}{|x - a_j|} \right)^{d_j}, \qquad x \in \Omega \subset \mathbb{R}^2 \simeq \mathbb{C},$$

for a harmonic phase function $H \in C^\infty(\overline{\Omega})$ such that the boundary conditions are satisfied.

Time interval

While GP is globally (in time) well-posed, the vortex dynamics is valid only up to the first vortex collision.

Objectives

Goal

Numerical simulation of (GPE) in the regime of small ε's.

- With standard methods (FEM, FD, FV...), $\varepsilon \ll 1$ typically requires very fine space/time discretization to avoid stability issues.
- Here, the well-known theory of vortex dynamics in the singular limit $\varepsilon \to 0$ can be used to circumvent these difficulties.
- Main idea: simulate the (finite dimensional) Hamiltonian dynamics (HD) instead of the (infinite dimensional) equation (GPE).

Jacobian estimates to localize the vortices

- Most of the convergence results are based on compactness arguments: no rate of convergence. . .
- Significant improvement in 2008, with estimate on $J\psi_\varepsilon$ and $j(\psi_\varepsilon)$ for small, but finite, ε:

Theorem (Jerrard, Spirn, 2008[6])

Let ψ_ε solve (GPE) *with well-prepared initial conditions, for some initial vortices with positions $\boldsymbol{a}^0 = (a_j^0)_{j=1,\dots,N}$ and degrees $(d_j)_{j=1,\dots,N}$. Then, there exists ε_0, $0 < \beta, \xi < 1$ and $C > 0$, depending only on Ω and the initial conditions, such that, for any $\varepsilon < \varepsilon_0$, well-preparedness is preserved along time. In particular,*

$$\text{(JS)} \qquad \left\| J\psi_\varepsilon(t) - \pi \sum_{j=1}^{N} d_j \delta_{a_j(t)} \right\|_{\dot{W}^{-1,1}} \lesssim \varepsilon^\beta \quad \text{and} \quad \left\| j(\psi_\varepsilon(t)) - j(u^*(\boldsymbol{a}(t), d)) \right\|_{L^{\frac{4}{3}}} \lesssim \varepsilon^\xi$$

for any $0 \le t \le \tau_{\varepsilon,\boldsymbol{a}^0}$, where $\boldsymbol{a}(t) = (a_j(t))_{j=1,\dots,N}$ solves the Hamiltonian ODE (HD) *and $\tau_{\varepsilon,\boldsymbol{a}^0}$ depends on ε and $\boldsymbol{a}^0$.*

[6] R. L. Jerrard and D. Spirn. Refined Jacobian Estimates and Gross–Pitaevsky Vortex Dynamics. *Archive for Rational Mechanics and Analysis*, 190(3):425–475, 2008.

Some comments on these results

- The $\dot{W}^{-1,1}$ is the good norm to use because

$$|a_i - b_i| \leqslant \frac{1}{4} \min_{j,k\neq j} \left\{ |a_j - a_k|, \mathrm{dist}(a_j, \partial\Omega) \right\} =: \rho_{\boldsymbol{a}} \quad \Rightarrow \quad \left\| \pi \sum_i d_i(\delta_{a_i} - \delta_{b_i}) \right\|_{\dot{W}^{-1,1}} = \sum_i \pi |d_i| |a_i - b_i|.$$

  $\rightsquigarrow$ not tractable numerically, better use the $L^{\frac{4}{3}}$ norm on the super-current.

- $\tau_{\varepsilon,\boldsymbol{a}^0}$ defined such that the result remains valid for times up to $O(\ln(1/\varepsilon))$ or the first vortex collision.
- Difficult and lengthy proof, the powers of ε appearing there are a bit arbitrary.

Well-prepared initial conditions

Well-prepared initial conditions

A family of initial conditions $(\psi_\varepsilon^0)_{\varepsilon>0}$ is said to be *well-prepared* if it satisfies the following assumptions, for some constant $C > 0$, $0 < \alpha < 1$ and ε small enough:

1. there exists N vortices with positions $\boldsymbol{a}^0 = (a_j^0)_{j=1,\dots,N} \in \Omega^N$ and degrees $d = (d_j)_{j=1,\dots,N} \in \{\pm 1\}^N$ such that

$$\left\| J\psi_\varepsilon^0 - \pi \sum_{j=1}^{N} d_j \delta_{a_j^0} \right\|_{\dot{W}^{-1,1}} \lesssim \varepsilon^\alpha,$$

   and the vortices are distant enough;

2. the energy of ψ_ε^0 is close to be optimal:

$$E_\varepsilon(\psi_\varepsilon^0) \leq \underbrace{W(\boldsymbol{a}^0, d) + N\left(\pi \ln(1/\varepsilon) + \gamma\right)}_{W_\varepsilon(\boldsymbol{a}^0, d)} + C\varepsilon^{\frac{1}{2}}.$$

$\rightsquigarrow$ the refined Jacobian estimates from JS'08 can be interpreted as the conservation of well-preparedness along time.

Numerical construction of well-prepared initial conditions

Well-prepared initial conditions can be obtained by smoothing out the harmonic canonical map u^* for a single vortex of degree $+1$[7]:

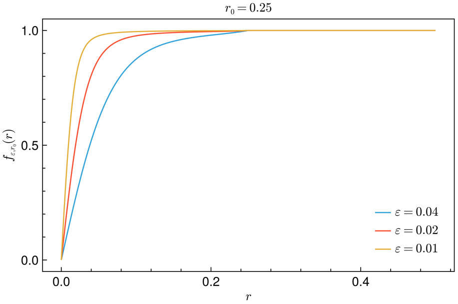
Make the ansatz $f(r)e^{\imath\theta}$ and insert it in the stationary equation $\Rightarrow f_{\varepsilon,r_0}$ has to solve, for a given $r_0 > 0$,

$$\frac{1}{r}\left(rf'_{\varepsilon,r_0}(r)\right)' - \frac{d^2}{r^2} f_{\varepsilon,r_0}(r) + \frac{1}{\varepsilon^2}\left(1 - |f_{\varepsilon,r_0}(r)|^2\right) f_{\varepsilon,r_0}(r) = 0,$$

with $f_{\varepsilon,r_0}(0) = 0$ and $f_{\varepsilon,r_0}(r_0) = 1$. Then, define

$$\psi^*_\varepsilon(x) = e^{\imath H(x)} \prod_{j=1}^{N} f_{\varepsilon,r_0}(|x - a_j^0|) \left(\frac{x - a_j^0}{|x - a_j^0|}\right)^{d_j},$$

where H is harmonic and such that $\partial_\nu \psi^*_\varepsilon = 0$.



[7] R. L. Jerrard and D. Spirn. Refined Jacobian Estimates and Gross–Pittaevsky Vortex Dynamics. *Archive for Rational Mechanics and Analysis*, 190(3):425–475, 2008.

- Such a family $(\psi_\varepsilon^*)_{\varepsilon>0}$ is well-prepared, for r_0 small enough.
- We also have the following results in terms of wave function and super-currents:

Lemma

Let $(\psi_\varepsilon^*)_{\varepsilon>0}$ be constructed as before. Then, for r_0 small enough, there exists some constant $C > 0$, independent of ε, such that

$$\|\psi_\varepsilon^*(\boldsymbol{a}, d) - u^*(\boldsymbol{a}, d)\|_{L^2} \leq C\varepsilon.$$

$$\left\|j\left(\psi_\varepsilon^*(\boldsymbol{a}, d)\right) - j(u^*(\boldsymbol{a}, d))\right\|_{L^p} \leq C(p)\varepsilon^{\frac{2}{p}-1} \quad \text{for } 1 \leq p < 2.$$

$\rightsquigarrow$ this typically implies that, for $p = \frac{4}{3}$, the power ξ of ε appearing in JS'08 is bounded by $\frac{1}{2}$.

1. Define initial vortex positions $\boldsymbol{a}^0 \in \Omega^N$ and degrees $d \in \{\pm 1\}^N$: define ψ_ε^0 by smoothing out the canonical harmonic map.
2. Evolve $\boldsymbol{a}(t)$ according to (HD) up to some maximum time T.
3. At time $t > 0$, build back an approximation of the solution ψ_ε from the vortex positions $\boldsymbol{a}(t)$ as

$$\psi_\varepsilon^*(t) = \psi_\varepsilon^*(\boldsymbol{a}(t), d) = u^*(\cdot; \boldsymbol{a}(t), d) \prod_{j=1}^{N} f_\varepsilon(|\cdot - a_j(t)|) \quad x \in \overline{\Omega},$$

where $u^*(x; \boldsymbol{a}(t), d)$ is the canonical harmonic map defined by

$$u^*(x; \boldsymbol{a}(t), d) = \exp(\imath H(x)) \prod_{j=1}^{N} \left(\frac{x - a_j}{|x - a_j|} \right)^{d_j},$$

with H the unique zero-mean harmonic function such that u^* satisfies the Neumann boundary conditions.

Warning

The harmonic function H is defined only up to a constant: this implies that the reconstructed wave function ψ_ε^* is an approximation of ψ_ε only up to a constant phase.

$$\begin{array}{ccc}
\text{initial conditions} & & \\
(\boldsymbol{a}^0, d) \in {\Omega^*}^N \times \{\pm 1\}^N & \xrightarrow[\text{(HD)}]{\text{evolve}} & (\boldsymbol{a}(t), d) \in {\Omega^*}^N \times \{\pm 1\}^N \\
\downarrow \text{smoothing} & & \text{smoothing} \downarrow \\
\text{well-prepared wave function} & & \\
\psi_\varepsilon^0 = \psi_\varepsilon^*(\boldsymbol{a}^0, d) & \xrightarrow[\text{(GPE)}]{\text{evolve}} & \psi_\varepsilon(t) \approx \psi_\varepsilon^*(\boldsymbol{a}(t), d) \qquad \text{(up to a constant phase)}
\end{array}$$

Figure: Diagram summarizing the numerical simulation of the GP equation via vortex tracking.

Mathematical justification

Let $\boldsymbol{a}^0 \in \Omega^{*N}$ and $d \in \{\pm 1\}^N$ be given as initial data. Let $\boldsymbol{a}(t)$ evolves according to (HD). Let ψ_ε be the solution to (GPE) with initial conditions $\psi_\varepsilon^0 = \psi_\varepsilon(\boldsymbol{a}^0)$ for ε and r_0 small enough. Then, for all $0 \leq t \leq \tau_{\varepsilon,\boldsymbol{a}^0}$,

1. Both $\psi_\varepsilon(t)$ and $\psi_\varepsilon^*(t)$ are close to be energetically optimal:

$$E_\varepsilon(\psi_\varepsilon(t)), E_\varepsilon(\psi_\varepsilon^*(t)) \leq W_\varepsilon(\boldsymbol{a}(t), d) + C\varepsilon^{\frac{1}{2}}.$$

2. Up to a constant phase, the error $\|\psi_\varepsilon(t) - \psi_\varepsilon^*(t)\|_{L^2}$ goes to 0 as $\varepsilon \to 0$.
3. The Jacobians and super-currents of ψ_ε and ψ_ε^* are close, in the sense

$$\|J\psi_\varepsilon(t) - J\psi_\varepsilon^*(t)\|_{\dot{W}^{-1,1}} \lesssim \varepsilon^\beta \quad \text{and} \quad \|j(\psi_\varepsilon(t)) - j(\psi_\varepsilon^*(t))\|_{L^{\frac{4}{3}}} \lesssim \varepsilon^\xi.$$

Proof: triangular inequalities together with the results from JS'08 and properties of the smoothing procedure. □

Recall the Hamiltonian ODE (HD)

$$\begin{cases} \dot a_j(t) = -\frac{1}{\pi} d_j \mathbb{J} \nabla_{a_j} W(\boldsymbol{a}(t), d), \\ a_j(0) = a_j^0, \end{cases} \quad \text{with} \quad \mathbb{J} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

for given initial positions $\boldsymbol{a}^0 \in \Omega^N$ and degrees $d \in \{\pm 1\}^N$. Here,

Boundary term $W_{\mathrm{bc}}(\boldsymbol{a}, d)$

$$\forall\ (\boldsymbol{a}, d) \in \Omega^N \times \{\pm 1\}^N, \quad W(\boldsymbol{a}, d) = -\pi \sum_{1 \le i \neq j \le N} d_i d_j \ln |a_i - a_j| - \pi \sum_{j=1}^N d_j R(a_j; \boldsymbol{a}, d),$$

with R the solution to

$$\begin{cases} \Delta R = 0 \quad \text{in } \Omega, \\ R = -\sum_{j=1}^N d_j \ln |x - a_j| \quad \text{on } \partial\Omega. \end{cases}$$

$$\begin{cases} \dot{a}_j(t) = -\frac{1}{\pi} d_j \mathbb{J} \nabla_{a_j} W(\boldsymbol{a}(t), d), \\ a_j(0) = a_j^0, \end{cases}$$

$$W(\boldsymbol{a}, d) = -\pi \sum_{1 \leq i \neq j \leq N} d_i d_j \ln |a_i - a_j| - \pi \sum_{j=1}^{N} d_j R(a_j; \boldsymbol{a}, d)$$

- Simulating the Hamiltonian system (HD) requires the evaluation of $\nabla_{a_j} W(\boldsymbol{a}, d)$. From BBH'94 [8] [Theorem VIII.3], it holds

$$\nabla_{a_j} W(\boldsymbol{a}, d) = -2\pi d_j \nabla_x \left(R(x; \boldsymbol{a}, d) + \sum_{i \neq j}^{N} d_i \ln |x - a_i| \right) \Bigg|_{x = a_j}.$$

- We are left with the resolution of a PDE at each time step to evaluate $\nabla_x R(x; \boldsymbol{a}, d)|_{x=a_j}$.

[8] F. Bethuel, H. Brezis, and F. Hélein. Ginzburg-Landau Vortices. *Birkhäuser Boston*, 1994.

Using harmonic polynomials to evaluate the renormalized energy

$$
\text{(R)} \qquad \begin{cases} \Delta R = 0 \quad \text{in } \Omega, \\ R = -\displaystyle\sum_{j=1}^{N} d_j \ln |x - a_j| \quad \text{on } \partial\Omega. \end{cases}
$$

- R is harmonic and the boundary condition is smooth as long as the vortices stay away from the boundary : we suggest to use harmonic polynomials.
- In the case where $\Omega \subset \mathbb{R}^2$ is the *unit disk*, the restriction of the harmonic polynomials to the boundary $\partial\Omega$ is nothing else than the basis of the Fourier modes for 2π-periodic functions.

1. Choose a maximum degree n and let $\mathbb{P}_n$ the $L^2(\partial\Omega)$-orthogonal projection operator from $L^2(\partial\Omega)$ to Fourier modes up to n: for any $g \in L^2(\partial\Omega)$,

$$(\mathbb{P}_n g)(e^{\imath\theta}) = \sum_{k=-n}^{n} \widehat{g}(k) e^{\imath k\theta}, \quad \text{where} \quad \widehat{g}(k) = \frac{1}{2\pi} \int_0^{2\pi} e^{-\imath k\theta} g(e^{\imath\theta}) d\theta.$$

2. Compute the Fourier coefficients $(\widehat{g}_a(k))_{-n\leq k\leq n}$ of the Dirichlet boundary condition in (R)

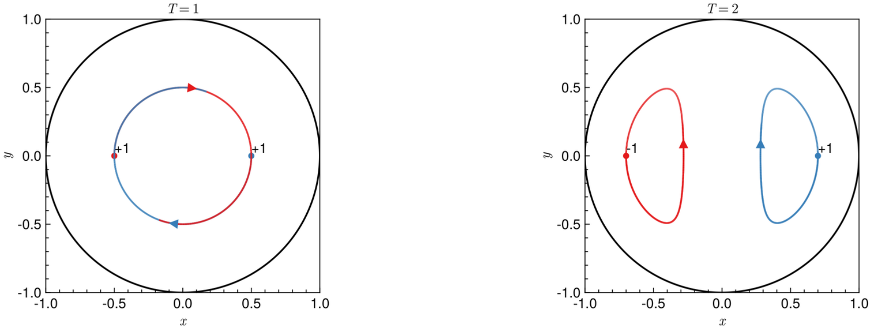
$$[0, 2\pi) \ni \theta \mapsto g_a(e^{\imath\theta}) := -\sum_{j=1}^{N} d_j \ln |(\cos\theta, \sin\theta) - a_j|$$

up to order n, for instance using a Fast Fourier Transform (FFT).

3. Compute the (approximate) solution R_n to (R) as the harmonic expansion of $\mathbb{P}_n g_a$:

$$\forall\ r \in [0, 1),\ \forall\ \theta \in [0, 2\pi), \quad R_n(re^{\imath\theta}) = \sum_{k=-n}^{n} r^{|k|} \widehat{g}_a(k) e^{\imath k\theta},$$

which is still harmonic by linear combination of harmonic functions.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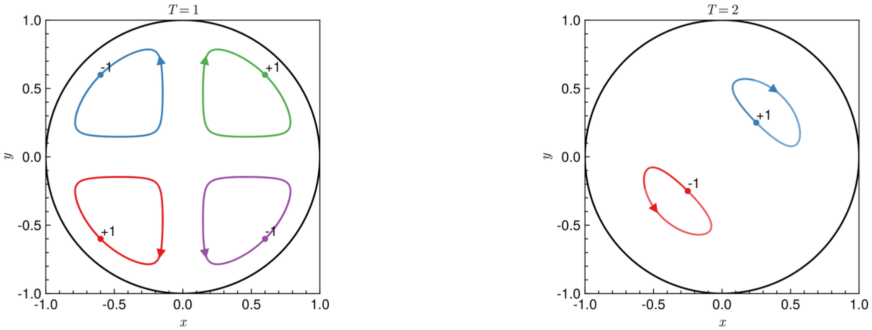
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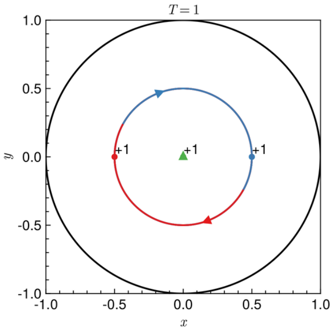
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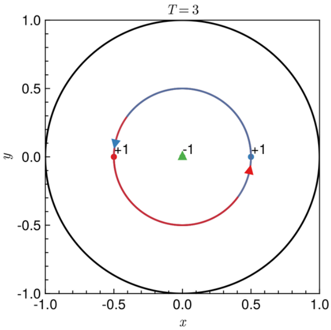
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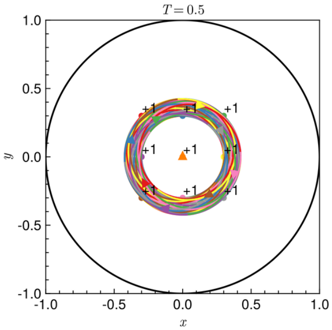

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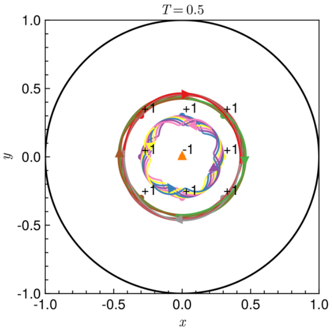

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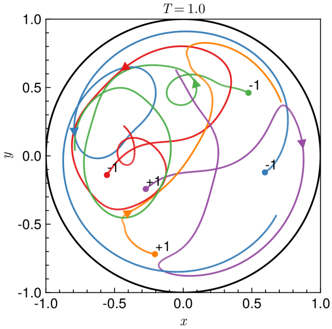
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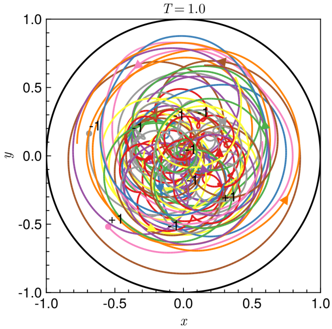
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-0.5
0.0
0.5
1.0
x
+1
-1
+1

Numerical simulation of the GPE *via* vortex-tracking

initial conditions $(\boldsymbol{a}^0, d) \in \Omega^{*N} \times \{\pm 1\}^N$	$\xrightarrow[\text{(HD)}]{\text{evolve}}$	$(\boldsymbol{a}(t), d) \in \Omega^{*N} \times \{\pm 1\}^N$
$\downarrow$ smoothing		smoothing $\downarrow$
well-prepared wave function $\psi_\varepsilon^0 = \psi_\varepsilon^*(\boldsymbol{a}^0, d)$	$\xrightarrow[\text{(GPE)}]{\text{evolve}}$	$\psi_\varepsilon(t) \approx \psi_\varepsilon^*(\boldsymbol{a}(t), d)$ (up to a constant phase)

Figure: Diagram summarizing the numerical simulation of the GP equation via vortex tracking.

Videos

Error control on the super-current

Error estimate on super-current

Let $\Omega \subset \mathbb{R}^2$ be the unit disk, and $\{\psi_\varepsilon(t)\}_{\varepsilon<\varepsilon_0}$ be the solution of (GPE) with well-prepared initial conditions for some initial vortices with positions $\boldsymbol{a}^0 = (a_j^0)_{j=1,\dots,N}$ and degrees $(d_j)_{j=1,\dots,N}$. Let $\boldsymbol{b}(t)$ be the approximated ODE trajectory with the same degrees and initial position $\boldsymbol{b}^0 = (b_j^0)_{j=1,\dots,N}$, with harmonic polynomials of degree up to n and time step δt with numerical integrator RK4. Let $\psi_\varepsilon^*(t)$ be the reconstructed wave function described above. Suppose that, for some $T > 0$,

$$\rho_T = \min_{t\leq T} \min\{|b_j(t) - b_k(t)|, \mathrm{dist}(b_k(t), \partial\Omega), |a_j(t) - a_k(t)|, \mathrm{dist}(a_j(t), \partial\Omega) : j \neq k\}$$

is such that $0 < \rho_T < 1$. Then there exists a constant $C > 0$ such that

$$\left\| j\big(\psi_\varepsilon^*(t)\big) - j\big(\psi_\varepsilon(t)\big) \right\|_{L^{\frac{4}{3}}(\Omega)} \lesssim_\ell \varepsilon^\xi + \frac{n^{-\ell+\frac{1}{2}}}{\rho_T^{\ell-\frac{1}{2}}} + \sqrt{\left(|\boldsymbol{a}^0 - \boldsymbol{b}^0| + \frac{(1-\rho_T)^n n^{1-\ell}}{\rho_T^{1+\ell}} T\right) \mathrm{e}^{Ct/\rho_T^{5/2}} + \delta t^4},$$

for any $t \in [0, T]$ and $\ell \in \mathbb{N}$.

Proof: at any time, split the error into

$$\|j(\psi_\varepsilon(t)) - j(\psi_\varepsilon^*(t))\|_{L^{\frac{4}{3}}} \leq \|j(\psi_\varepsilon(t)) - j(u^*(\boldsymbol{a}(t), d))\|_{L^{\frac{4}{3}}} + \left\|j\left(u^*(\boldsymbol{a}(t), d)\right) - j\left(u^*(\boldsymbol{b}(t), d)\right)\right\|_{L^{\frac{4}{3}}} + \left\|j\left(u^*(\boldsymbol{b}(t), d)\right) - j(\psi_\varepsilon^*(t))\right\|_{L^{\frac{4}{3}}},$$

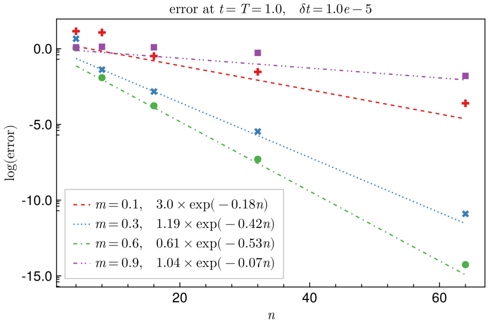
with $\boldsymbol{a}(t)$ the exact vortex trajectories and $\boldsymbol{b}(t)$ the approximated ones. Deal with each term separately:

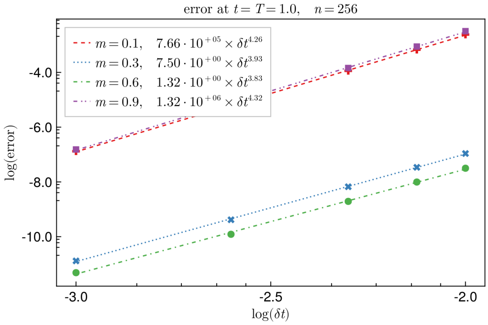
1. treated by JS'08,
2. needs more work: approximated resolution of (HD) (approximation of R and time integration)
   - RK4 numerical integrator yields δt^4,
   - harmonic polynomials yields spectral accuracy,
3. treated by the smoothing procedure, with additional error coming for the computation of the harmonic phase H, still with harmonic polynomials.

NB: the $\sqrt{\cdot}$ comes from the $\frac{4}{3}$ norm on the super-currents. □

Numerical convergence of the vortex trajectories

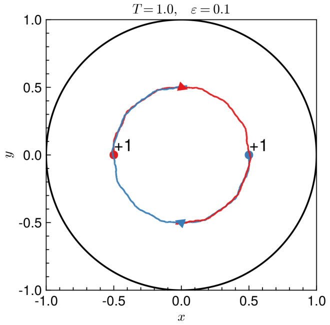
- Initial conditions given by $d = (+1, +1)$ and $\boldsymbol{a}^0 = (+m, 0), (-m, 0)$.
- Error on a reference, converged, trajectory *vs* an approximated one: $|\boldsymbol{a}(t) - \boldsymbol{b}(t)|$.

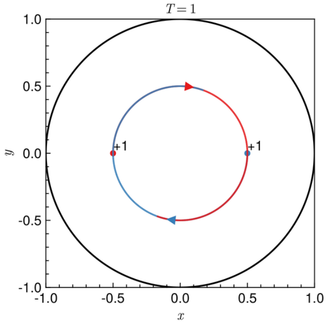




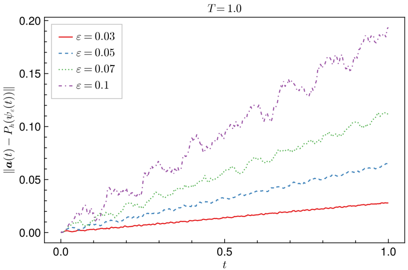
Numerical convergence of the vortex-tracking method

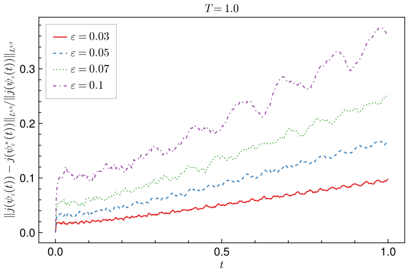
- Initial vortex location given by $d = (+1, +1)$ and $\boldsymbol{a}^0 = (+0.5, 0), (-0.5, 0)$.
- Run a reference, expensive, calculation to compute the solution to (GPE) with ψ_ε^0 as initial data for several ε's (we used `Gridap.jl`, a `Julia` FE solver).
- Compare different quantities: vortex trajectories[9], solutions in L^2 and H^1 norms, super-currents.

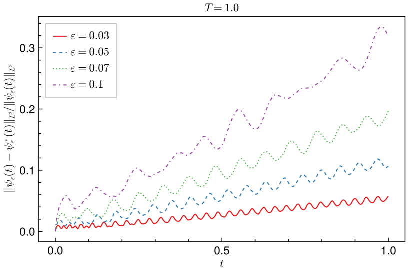


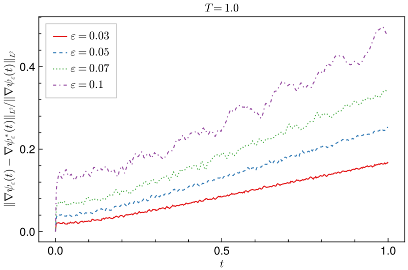


[9] W. Bao and Q. Tang. Numerical Study of Quantized Vortex Interactions in the Non-linear Schrödinger Equation on Bounded Domains. *Multiscale Modeling & Simulation*, 12(2):411–439, 2014.


$T = 1.0$
$\|\boldsymbol{a}(t) - P_h(\psi_\varepsilon(t))\|$
t
$\varepsilon = 0.03$
$\varepsilon = 0.05$
$\varepsilon = 0.07$
$\varepsilon = 0.1$
0.00
0.05
0.10
0.15
0.20
0.0
0.5
1.0

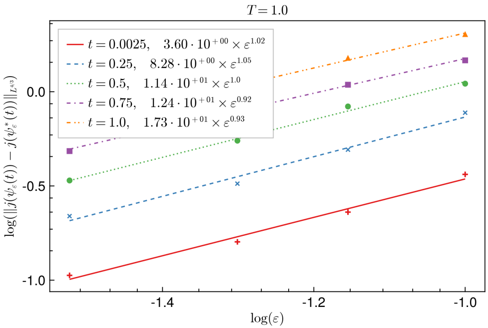

$T = 1.0$
$\|j(\psi_\varepsilon(t)) - j(\psi_\varepsilon^*(t))\|_{L^{4/3}}/\|j(\psi_\varepsilon(t))\|_{L^{4/3}}$
t
$\varepsilon = 0.03$
$\varepsilon = 0.05$
$\varepsilon = 0.07$
$\varepsilon = 0.1$
0.0
0.1
0.2
0.3
0.0
0.5
1.0

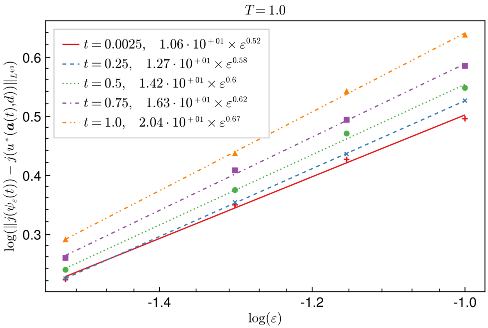

$T = 1.0$
$\|\psi_\varepsilon(t) - \psi_\varepsilon^*(t)\|_{L^2}/\|\psi_\varepsilon(t)\|_{L^2}$
t
$\varepsilon = 0.03$
$\varepsilon = 0.05$
$\varepsilon = 0.07$
$\varepsilon = 0.1$
0.0
0.1
0.2
0.3
0.0
0.5
1.0


$T = 1.0$
$\|\nabla\psi_\varepsilon(t) - \nabla\psi_\varepsilon^*(t)\|_{L^2}/\|\nabla\psi_\varepsilon(t)\|_{L^2}$
t
$\varepsilon = 0.03$
$\varepsilon = 0.05$
$\varepsilon = 0.07$
$\varepsilon = 0.1$
0.0
0.2
0.4
0.0
0.5
1.0

Numerical study of ε's powers

$$\left\| j\big(\psi^*_\varepsilon(t)\big) - j\big(\psi_\varepsilon(t)\big) \right\|_{L^{\frac{4}{3}}(\Omega)} \lesssim_\ell \varepsilon^\xi + \frac{n^{-\ell+\frac{1}{2}}}{\rho_T^{\ell-\frac{1}{2}}} + \sqrt{\left(|\boldsymbol{a}^0 - \boldsymbol{b}^0| + \frac{(1-\rho_T)^n n^{1-\ell}}{\rho_T^{1+\ell}} T \right) \mathrm{e}^{Ct/\rho_T^{5/2}} + \delta t^4}$$





Take-home message:

- The well-known analytical framework of the singular limit $\varepsilon = 0$ permits a numerical method which is more accurate as $\varepsilon \to 0$, in contrast to standard methods.
- Well-preparedness being preserved over time, we can recover an approximation in H^1 (while $u^* \notin H^1$).
- Error control on the super-current in $L^{\frac{4}{3}}$ is possible, the smoothed out approximation ψ_ε^* seems to give an exponent of order 1 to ε while, as expected, the canonical harmonic map is limited to $\frac{1}{2}$.
- Limits: nonlinear phenomena such as radiation waves emitted by vortex collision cannot be reproduced. . . (BT'14).

Perspectives:

- Easy extension to unknown vortex locations in the initial wave function.
- Sharpness of the error bound ?
- Learning vortex trajectories with machine learning (recent works on Hamiltonian neural networks):
  - Knowing the real Hamiltonian makes validation easier.
  - Extension to models of vortices where the Hamiltonian is unknown (with magnetic fields ?).

Merci !

https://arxiv.org/abs/2404.02133

Joint works with

Benjamin Stamm
(Univ. Stuttgart)

Christof Melcher
(RWTH Aachen)

Thiago Carvalho Corso
(Univ. Stuttgart)