The Gross-Pitaevskii equation (GPE): Dynamics of solitons and vortices

Thorsten Buss and Jeremias Traub and Jeremias Gutekunst

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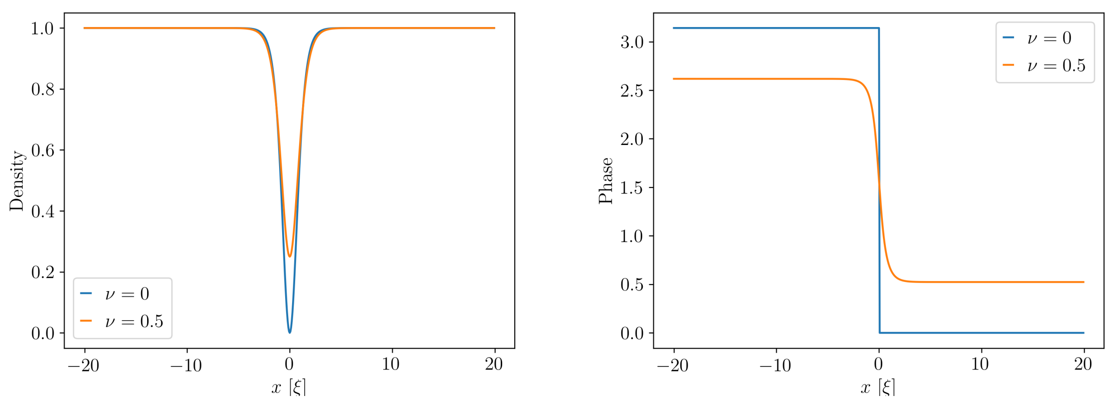
1 Introduction

This work addresses the topic of soliton and vortex dynamics in the framework of the Gross-Pitaevskii equation (GPE) using simulation models. It was carried out as part of the lecture *Computational Quantum Dynamics* (Dr. M. Gärttner, WS19/20). The experimental realization and motivation of these simulations are Bose-Einstein-Condensates (BEC), that can be formed in magneto-optical traps. The BEC can be formed into cigarre-shapes or planes using additional Fields. This correspondents to the 1d and 2d setups in the simulations. BEC's are of particular interest in current research as they show quantum mechanical behavior on a macroscopic scale.

2 Theoretical Background



(a) Density profile

(b) Phase profile

Figure 1: Phase (*left*) and density (*right*) profiles for a black soliton ($\nu = 0$) and a grey soliton with $\nu = 0.5$.

It was found that the Gross-Pitaevskii-Equation (GPE) is very successful in describing BEC's. It is a non-linear Partial-Differential-Equation (PDE) and describes the time evolution of the mutual wavefunction of the bosons in the condensate:

$$\Big[-\frac{\hbar^2\nabla^2}{2m} + V(r) - \mu + g\phi\phi^*\Big]\phi = -ih\partial_t\phi \tag{1}$$

Here, the interaction strength g is positive for repelling interactions and negative for attractive interactions of the bosons. μ is the chemical potential and V is an arbitrary potential which we will set to zero in the following. Further we choose $g = 1$, i.e. repelling interactions, for all simulations.

Solitons are non-dispersive solutions of the GPE. For $V = 0$ and by setting most of the parameters such as the background density n and the chemical potential μ to 1, they are of the following form:

$$\phi(x,t) = \left[i\nu + \gamma^{-1} \tanh\left(\frac{x - (x_0 + \nu t)}{\gamma} \right) \right] \exp^{it} \tag{2}$$

Hereby, $\nu = v_s/c_s$ where v_s is the velocity and c_s the Bogoliubov speed of sound. The Lorentz factor γ^{-1} is given by $\sqrt{1-\nu^2}$. In Eq.2 the unit of length is the healing lenght ξ, and the unit time becomes $\tau := \xi/c_s$.

Solitons are essentially characterized by two parameters: the starting point x_0 and ν which determines the speed, phase shift and greyness of the soliton. In the special case of $\nu = 0$ the soliton is called *black*. Fig.1a shows the density profile of the Bose field for two different values of ν, Fig.1b shows the respective phase profiles.

3 Split-step Fourier Method

In order to propagate the wavefunction in time we apply the split-step fourier method (SSFM). It exploits the fact that the kinetic term of the hamilton operator is diagonal in momentum space and that an arbitrary potential which can be time dependent (here: $g\phi\phi^*$) is diagonal in real space. We switch back and forth from real space to momentum space using the Fourier-transformation. Then we propagate the state in the two spaces using the potential part and the kinetic part of the hamiltonian, respectively. For small time steps dt the following equation holds:

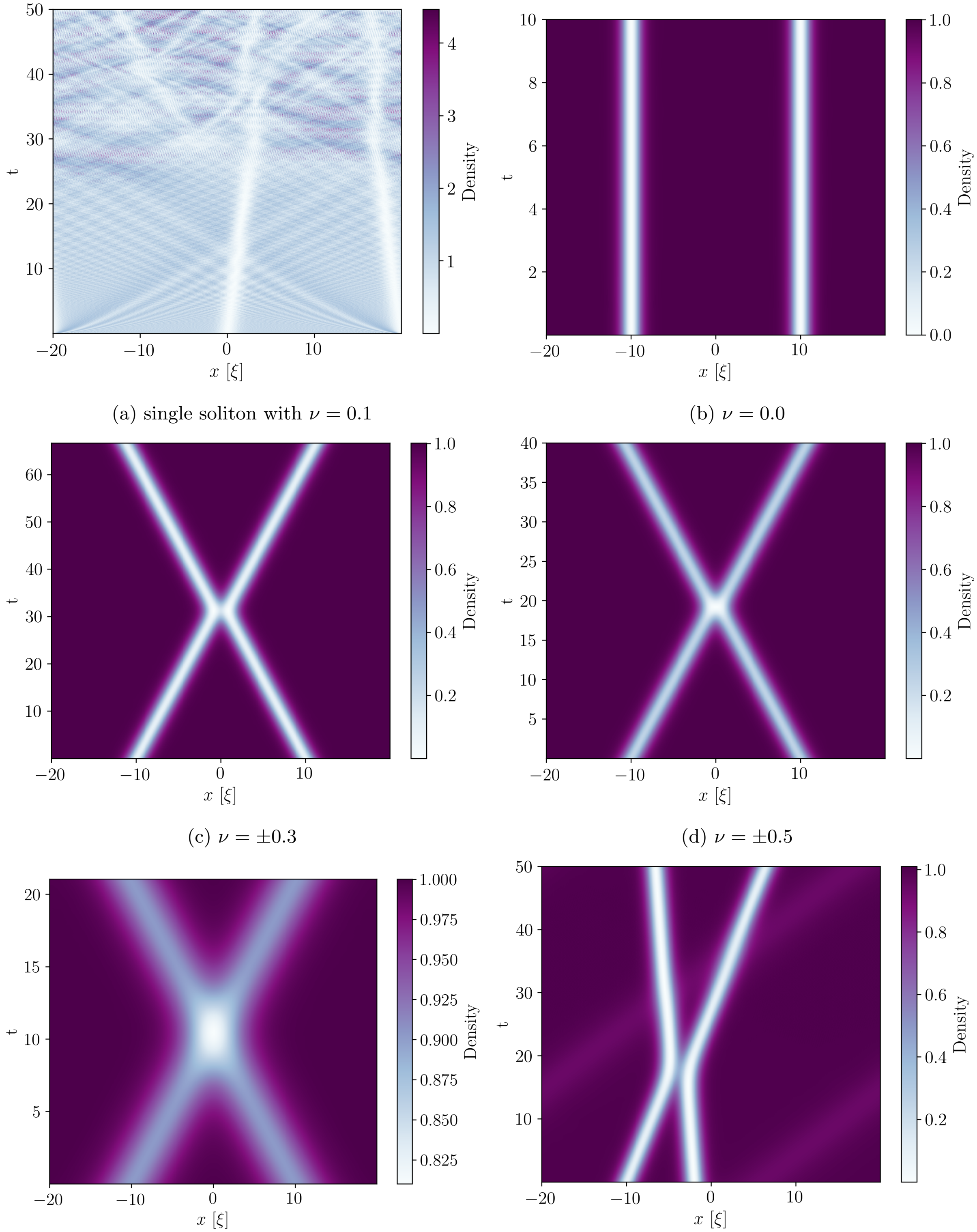
$$\begin{aligned} U(H(t)) &= e^{-idtH(t)} = e^{-idt(H_{kin}+H_{pot}(t))} = e^{-idtH_{kin}} e^{-idtH_{pot}(t)} \\ &= F^{-1}Fe^{-idtH_{kin}}F^{-1}Fe^{H_{pot}(t)} = F^{-1}e^{-idtD_{kin}}Fe^{H_{pot}(t)} \end{aligned} \tag{3}$$

F represent the Fourier-transformation, F^{-1} the backtransformation. If we choose to represent our state in real space the potential term is already diagonal, the kinetic term becomes diagonal after the transformation. Applying Eq.3 iteratively then yields the SSFM.

4 Simulation of Solitons in 1 Dimension

In order to simulate solitons in one dimension we choose a grid with a cell size smaller than the characteristic healing length $\xi = 1$. We choose a domain size of 40 resolved by 600 grid points. The time step size is set to 0.01.

As we study the time evolution of solitons on a grid with periodic boundary conditions *automatically* imposed by the SSFM, we need to simulate at least two solitons. If one would only simulate a single soliton, there would be a phase jump at the boundary which would cause unwanted side effects. This was done in Fig. 6a. One can see, that the phase jump at the boundary provokes a soliton-like behavior. The "second soliton" which is generated at the boundary has the opposing velocity or greyness. This corresponds to a phase-jump that compensates for the original soliton. Consequently, we need to simulate at least two solitons with $\nu_1 = -\nu_2$. When simulating 3 solitons we have the freedom to choose two of the ν's independently.



(a) single soliton with $\nu = 0.1$

(b) $\nu = 0.0$

(c) $\nu = \pm 0.3$

(d) $\nu = \pm 0.5$

(e) $\nu = \pm 0.95$

(f) $\nu_1 = 0.3$, $\nu_2 = -0.05$, $\nu_3 \approx 0.97$

Figure 2: Temporal development of the density profile for different initial configurations. *(a)* A single soliton causes unwanted boundary effects; *(b)* Black solitons; *(c)*-*(e)* Two solitons with increasing ν; *(f)* Three solitons.

In Fig.6b one can see the time evolution of black solitons which are stationary. We tried configurations of two solitons with opposite ν for different values of ν to test collisions of grey solitons. For $|\nu| < 0.3$ the solitons stay distinguishable (see Fig.6b - 6c), they repel each other [1]. The momentum of the solitons appears to be conserved as it is transferred from one soliton to the other. In Fig.6d, for $|\nu| = 0.5$, the solitons overlap and part afterwards. As we set ν to even higher absolute values the solitons overlap even more (see Fig.6e). In the particle model one can no longer distinguish the two solitons after the collision. In Fig.6f 3 solitons are simulated. The slow (darker) solitons stay distinguishable and exchange their impulses as they collide. The fast soliton overlaps with the slower ones as it crosses their trajectories.

5 Simulation of Solitons in 2 Dimensions

We now study the dynamics of solitons in a homogeneous 2D Bose gas. Hence, we consider a two-dimensional regular periodic grid. We choose a grid size of (16×16) (in units of the healing length ξ) with each dimension being resolved by 256 grid cells.

In two dimensions, a simple soliton is given by the one-dimensional solution (see Eq.**??**) in one direction uniformly extended in the other direction, i.e., $\phi(x, y, t) = \phi(x, t)$. As in the 1d case, at least two solitons are needed in order to respect the periodic boundary condition.

We initialize two solitons at the locations $x = \pm 10$ (compare Fig.3a - 3b). We notice that without any noise the two solitons are a (meta-)stable solution and do not change over the simulation time of 70τ. For $|\nu| > 0$, i.e. for moving solitons, we make the same observations as in the 1d case (not shown here).

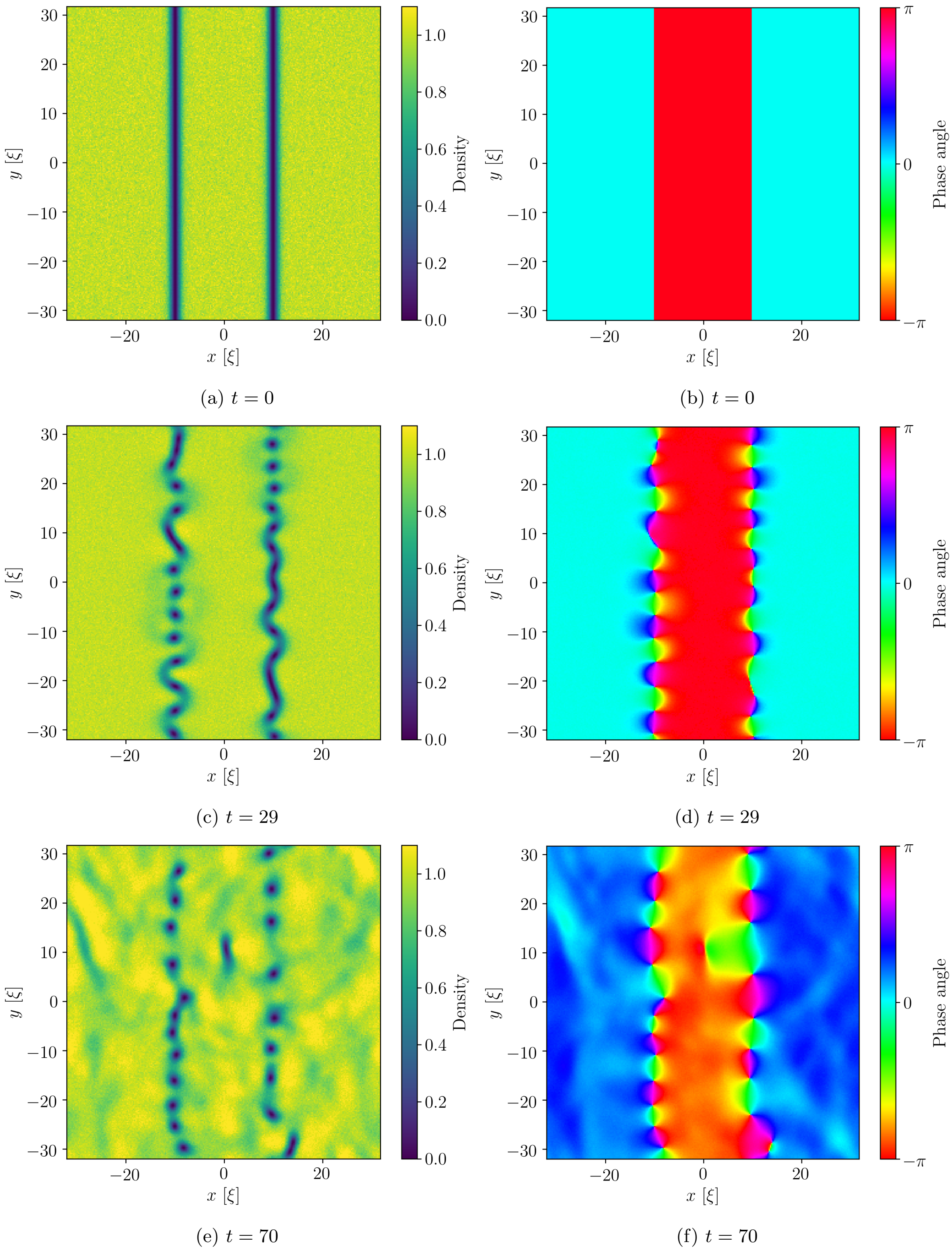
In order to test the stability of the initial states we add normally distributed noise to it, in the way that we multiply each grid value by a random number drawn from $\mathcal{N}(\mu = 1, \sigma = 0.02)$[1].

Fig.3 shows the temporal development of both density and phase. After a certain *ramp-up* time[2] in which instabilities grow, the line structure breaks down to single-quantized vortex-antivortex pairs (note the periodic phase pattern in Fig.3d) which move and cluster as time increases (see Fig.3c - 3f). An animation can be found on the project page.

Next, we consider a configuration where the qualitative dynamics of the 1d case – even with noise – is recovered. We initialize a ring-like soliton (see Fig.4a) with a greyness of $\nu = -0.5$, i.e. a contracting ring. Fig.4 shows the temporal development. One can see that the ring contracts until a critical point in time is reached after which it starts to expand. The phase jumps by $\pm\pi$. We identify the turning point at $\phi = \pm\pi$ (see Fig.4d).

[1] In order to generate something like *thermal* noise one would rather add random numbers drawn from $\mathcal{N}(\mu = 0, \sigma)$. Here, however, we are only interested in small disturbances that initialize a quick decay of the solitons.

[2] The length of this phase particularly depends on the amplitude of the noise.

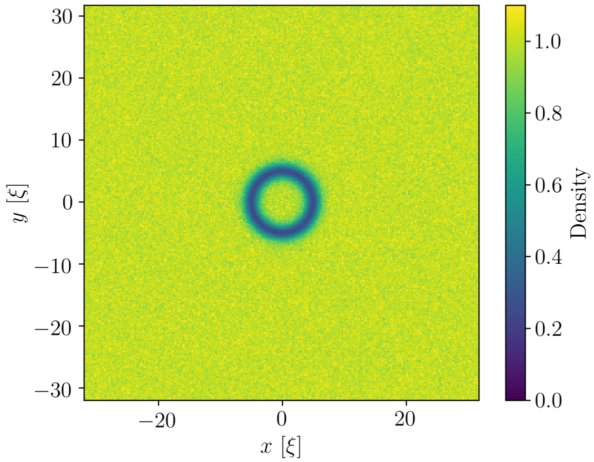


(a) $t = 0$ (b) $t = 0$

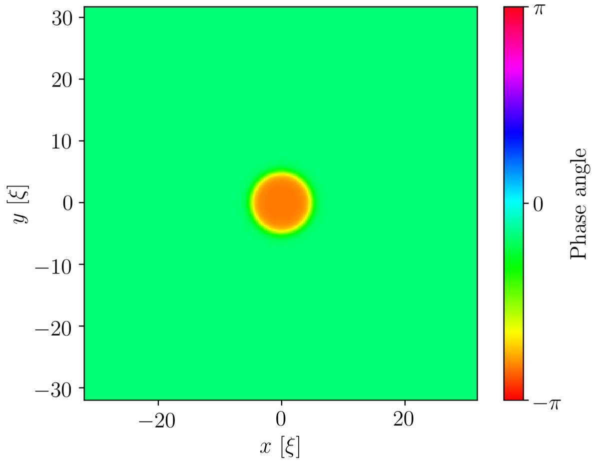
(c) $t = 29$ (d) $t = 29$

(e) $t = 70$ (f) $t = 70$

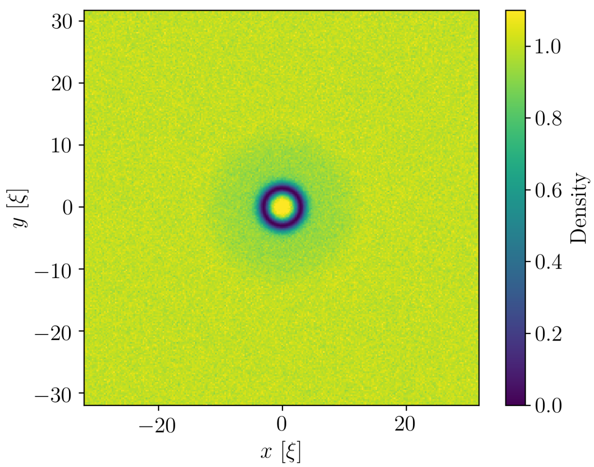
Figure 3: Temporal development of 2 solitons in a 2d BEC. The density (*left* column) and the phase (*right* column) distributions are shown for the times $0, 29, 70$. Noise is added to the initial state which allows for growing instabilities in the *ramp-up* phase. The line structure then breaks down to single-quantized vortex-antivortex pairs.



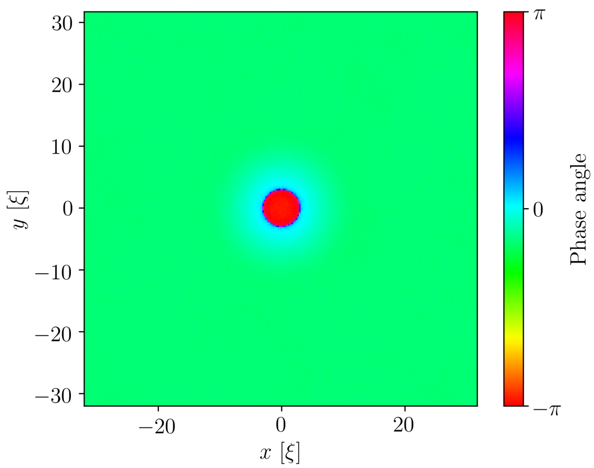
(a) $t = 0$



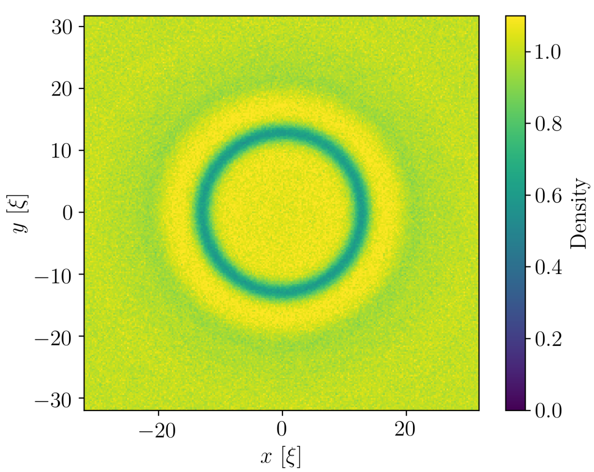
(b) $t = 0$



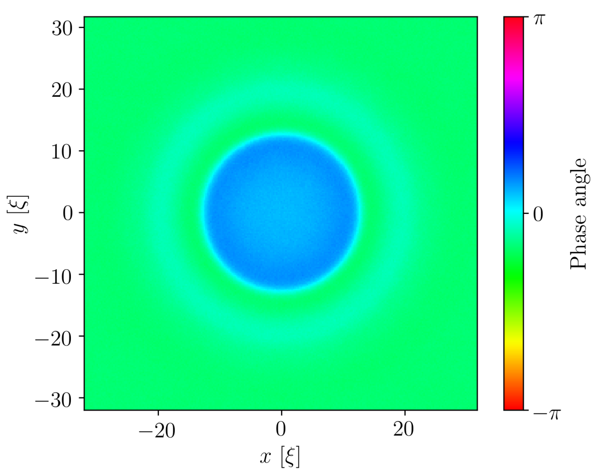
(c) $t = 5.6$



(d) $t = 5.6$



(e) $t = 20$



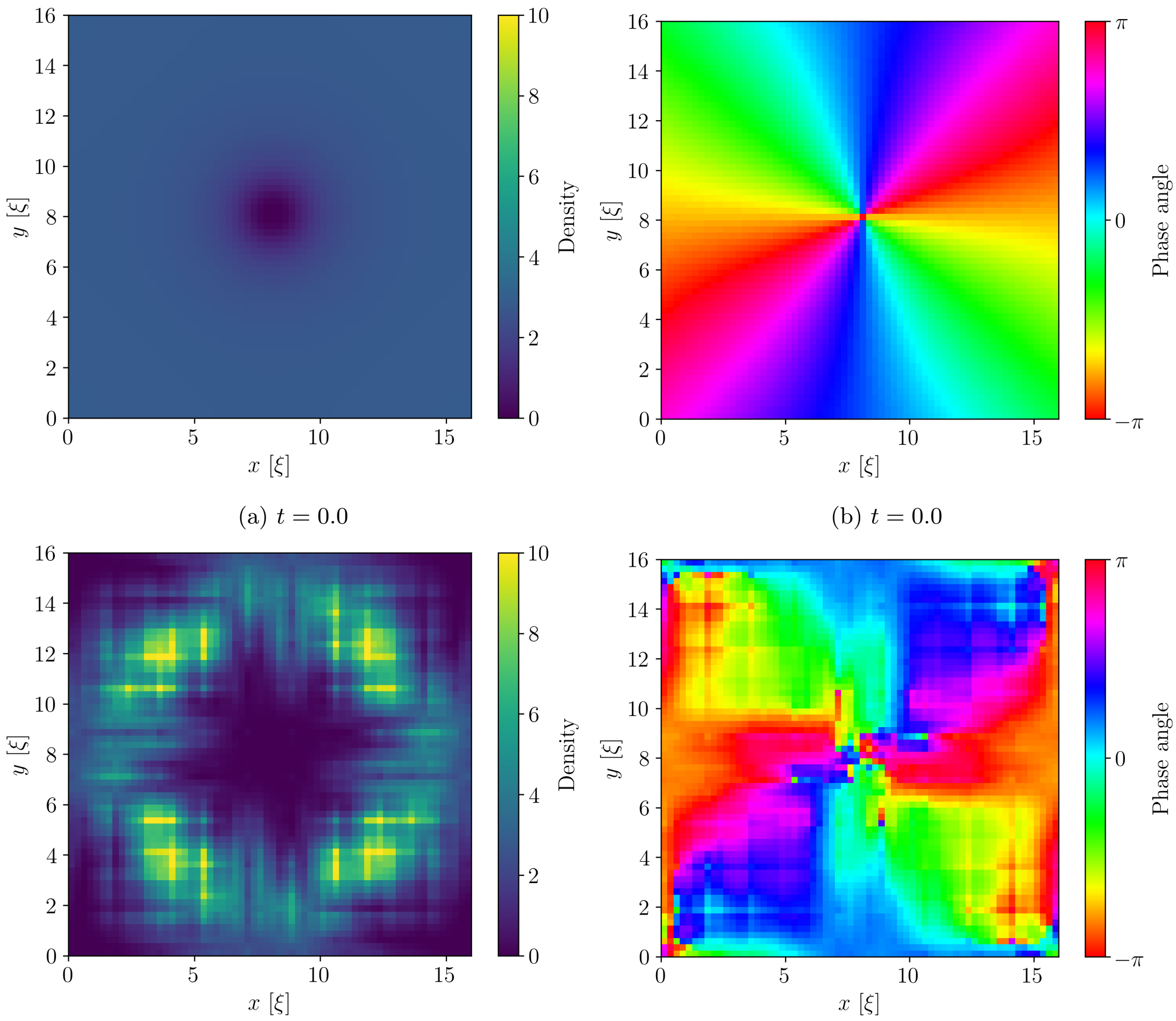
(f) $t = 20$

Figure 4: Temporal development of a ring-like solitons in a 2d BEC; intitialized with radius of $R = 5$ and greyness $\nu = -0.5$. The density (*left* column) and the phase (*right* column) distributions are shown for the times $0, 5.6, 20$. The configuration exhibits the same qualitative dynamics as in the 1d case.

6 Simulation of Vortices in 2 Dimensions

We now study the dynamics of vortices in a homogeneous 2D Bose gas. Hence, we again consider a two-dimensional regular periodic grid. We choose a grid size of (16×16) (in units of the healing length ξ) with each dimension being resolved by 64 grid cells.

A vortex is a solution of the GPE. It is a density dip, with the phase changing by $2n\pi$ while moving around the dip. They already appeared in the previous section, when the 2D-Solitons decayed into pairs of vortices with $n = 1$ and anti-vortices with $n = -1$. In the following we study the behavior of a single vortex and that of vortices on a lattice with winding number $n = \pm 4$.



(a) $t = 0.0$ (b) $t = 0.0$

(c) $t = 4.0$ (d) $t = 4.0$

Figure 5: Temporal development of a single vortex with quantization $n = 2$. The periodic boundaries force an anti-vortex-like structure to emerge.

When initializing a single vortex it is impossible to respect the periodic boundaries. Consequently, there will be a phase jump at the boundary which again results in the creation of a vortex-like phenomenon. In Fig.5 one can see that the initial condition of a vortex with $n = 2$ causes boundary effects that provoke a density dip which is displayed in all four corners of the grid (which is actually only one region) circled by a phase structure that would fit to a vortex with $n = -2$, i.e. an anti-vortex to the initial one.

In Fig.6 vortices with $n = 4$ are initially arranged on a regular lattice. The vortex positions have a random offset. As for the solitons in 2d disturbances are needed in order for the regular structure to decay. In the case of a perfect regular lattice we observe stable periodic cycles. An animation can be found on the project page.

With offsets, the vortex structure is unstable as the vortices break up into smaller scaled clusters. Patches of similar phase seem to emerge. At the boarders of those areas are trenches in the density distribution. In [2] the authors could simulate a behavior where these patterns further developed into a vortices with $n = \pm 1$. Apparently opposing vortices annihilated each other after a certain time. Even though we observe similar behavior, we could not reproduce their results. However we used a much lower spatial resolution and less time steps as we were limited in computational power. An animation of the simulation can be found on the project page.

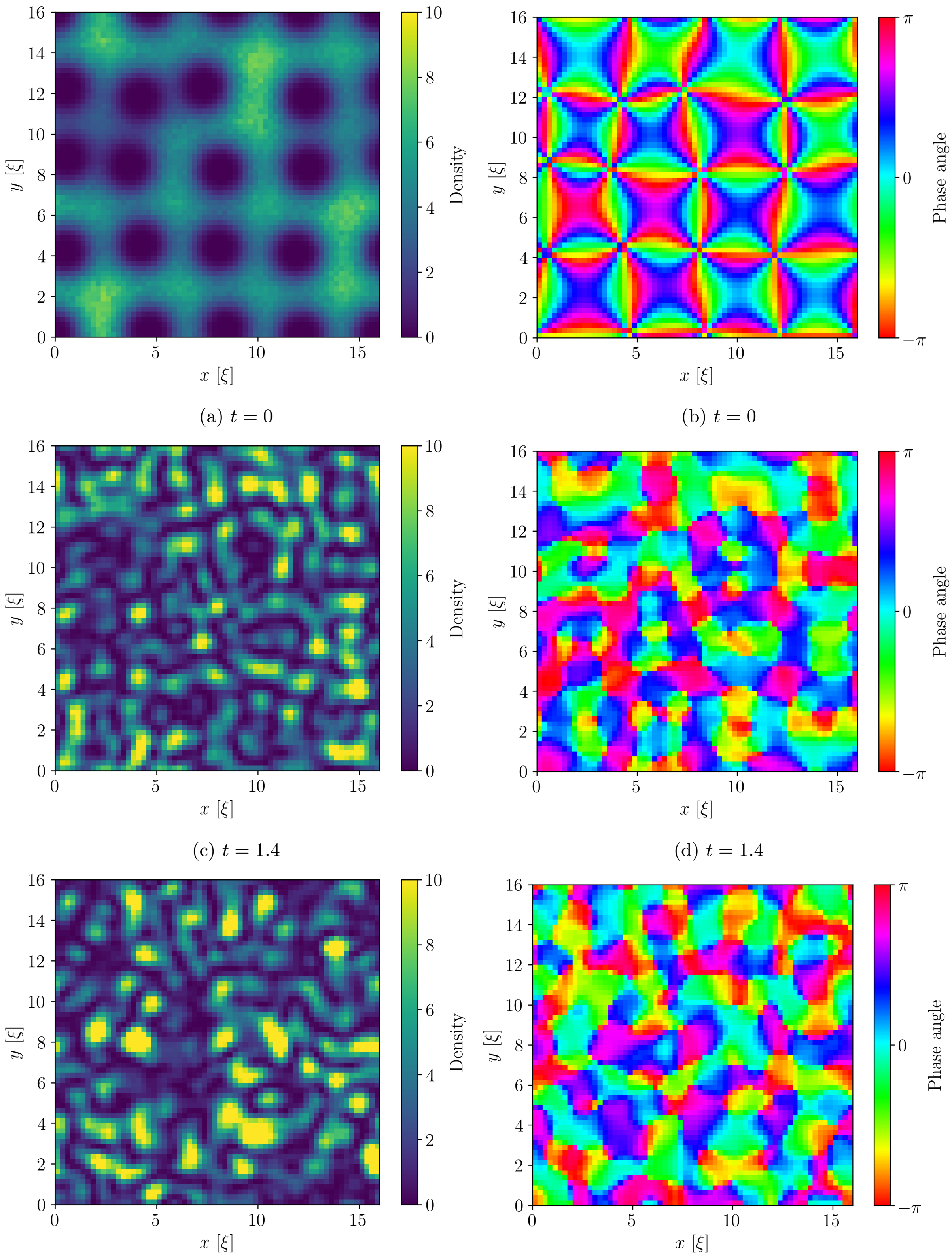
7 Summary

We modelled the dynamics of solitons and vortices in a BEC represented by one-dimensional and two-dimensional grids. We provide three models (see our project page) that allow for easy configuration and use. With that, we were able to reproduce parts of the results in [1] and [2].

References

[1] Thomas Gasenzer Sebastian Erne. Characterization of solitonic states in a trapped ultracold bose gas. Master's thesis, University of Heidelberg, 2012.

[2] Gunjan Verma, Umakant D Rapol, and Rejish Nath. Snake instability and the emanating vortex dynamics in two dimensional matter wave dark solitons. *gas*, 2016.



(a) $t = 0$ (b) $t = 0$

(c) $t = 1.4$ (d) $t = 1.4$

(e) $t = 6.0$ (f) $t = 6.0$

Figure 6: Temporal development of vortices with $n = 4$ initially arranged on a regular lattice with random offsets. The vortices decay into lower-quantized vortices.