The Gross-Pitaevskii equation: Dynamics of solitons and vortices

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The Gross-Pitaevskii equation is a mean field equation that has been incredibly successful in describing the dynamics of Bose-Einstein condensates. The equation features a non-linear term and thus allows for stable soliton solutions in 1D and additional topological defects such as vortices in 2D. The goal of this project is to study these phenomena using the Split-Step Fourier method.

Remark: This report summarizes the results of the final project we conducted as part of the lecture course on Computational Quantum Dynamics, held by Dr. Martin Gärttner at Heidelberg University during the winter term 2018/2019. All numerical work was done using the Python programming language.

1 Introduction

In the first part of this report we want to present the physical concepts needed for the understanding of the performed calculations. At the end, the Split-Step Fourier method, which we used to analyze the dynamics of the different quantum systems, is introduced.

The Gross-Pitaevskii equation (GPE) successfully describes the dynamics of Bose-Einstein condensates. Here, we want to introduce the corresponding physical situation, along with its assumptions.

1.1 Bose-Einstein condensation

Bose-Einstein condensates (BECs) are states of matter of dilute boson gases cooled down to temperatures very close to absolute zero.
The most important characteristic of such system is, that a large fraction of bosons occupies the lowest quantum state. Although one would assume that the understanding of the dynamics of a BEC is based on the microscopic, i.e. the quantum-mechanical, properties of the single bosons forming the gas, it is possible to describe Bose-Einstein condensates with one single, macroscopic wave function $\psi(\mathbf{r}, t)$.
For an exact description of N interacting quantum particles we would need the N-body wavefunction, $\psi(r_1, r_2, ...r_N, t)$, which obeys the many-body Schrödinger equation. We assume the interactions between the particles to be very weak, which is well-founded in the diluteness of the gases and the weak forces between neutral atoms. By neglecting the effects of quantum fluctuations, the many-body wave function for large particle numbers ($N \gg 1$) is replaced by an *effective* single-particle wave function $\psi_{\text{eff}}(\mathbf{r}, t)$.
In a field-theoretical approach to the subject, one would introduce this macroscopical wave function as a complex field of the form

$$\psi_{\text{eff}}(\mathbf{r}, t) = \sqrt{n} \cdot \exp\left(\frac{i}{\hbar}\, \mathcal{S}(\mathbf{r}, t)\right) \tag{1}$$

with the density and phase distributions n and $\mathcal{S}$ of the condensate. It is normalized to the particle number N, such that

$$\int \mathrm{d}^3\mathbf{r}\, \|\psi\|^2 = N. \tag{2}$$

1.2 From the Schrödinger equation to the GPE

For an ideal Bose gas, i.e. without interactions between the particles, the evolution of the system over time would be governed by the time-dependent Schrödinger equation

$$i\hbar\, \frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\psi(\mathbf{r},t) \tag{3}$$

with the Laplacian ∇^2 and the potential $V(\mathbf{r},t)$.
One needs to modify this equation to include the particle interactions to describe the physical situation more precisely. We assume that elastic next-neighbor interactions between two single particles due to Van-der-Waals forces dominate the interaction processes inside the gas. This allows us to describe these processes using the model of hard-sphere interactions, which yields

$$\mathcal{U}(\mathbf{r_1},\mathbf{r_2}) = g_{3D}\cdot\delta_D(\mathbf{r_1}-\mathbf{r_2}) \tag{4}$$

for the interaction potential, where the interaction strength g_{3D} is defined as

$$g_{3D} = \frac{4\pi\hbar^2 a_s}{m} \tag{5}$$

with the scattering length a_s in the low-energy limit.
Taking these interactions into accounts yields us to the modified, nonlinear version of the Schrödinger equation, the *Gross-Pitaevskii equation*

$$i\hbar\, \frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t) + g\|\psi\|^2\right]\psi(\mathbf{r},t). \tag{6}$$

All numerical calculations in this project are based on this equation.

Some words on the Bogoliubov mean-field approach: Working with field operators $\hat{\psi}$, induced by equation (1) leads us to a Hamiltonian description of the situation with the grand canonical Hamiltonian, here in one spatial dimension

$$\hat{\mathcal{H}} = \int \mathrm{d}z\, \hat{\psi}^\dagger(z)\left[-\frac{\hbar^2}{2m}\partial_z^2 + V(z) - \mu + \frac{g_{1D}}{2}\hat{\psi}^\dagger(z)\hat{\psi}(z)\right]\hat{\psi}(z) \tag{7}$$

where g_{1D} is the interaction parameter for one dimension and μ is the chemical potential. Choosing suitable parameters for the spatial grid structure, one finds solutions for the discretized version of the GPE from this approach as

$$\left[-\frac{\hbar^2}{2m}\partial_z^2 + V(z) - \mu + g_{1D}\, n\right]\sqrt{n} = 0. \tag{8}$$

The following two sections introduce topological defects in one and two spatial dimensions, namely solitons and vortices, which are analyzed numerically later on.

1.3 Solitons

Solitons are non-dispersive wave solutions of the Gross-Pitaevskii equation. In the following we distinguish between bright solitons, describing attractive interactions and dark solitons for repulsive interactions. The latter ones will be the objects of interest for our studies. They are characterized by their so called *greyness* $\nu = {}^{v_s}/_{c_s}$ with the Bogoliubov speed of sound $c_s = \sqrt{{}^{ng}/_{m}}$ and the velocity v_s of the solitons movement inside the gas.
If we restrict ourselves to the case of repulsive interactions and a vanishing external potential, the analytic solution for a single solitonic excitation reads

$$\phi_\nu^{(1)}(z,t) = \sqrt{n}\left[i\nu + \gamma^{-1}\tanh\left(\frac{z-(z^0+\nu c_s t)}{\sqrt{2}\xi\gamma}\right)\right]\mathrm{e}^{i\mu t} \tag{9}$$

with the Lorentz factor $\gamma^{-1} = \sqrt{1-\nu^2}$ and the healing length $\xi = {}^{1}/_{\sqrt{mng}}$.

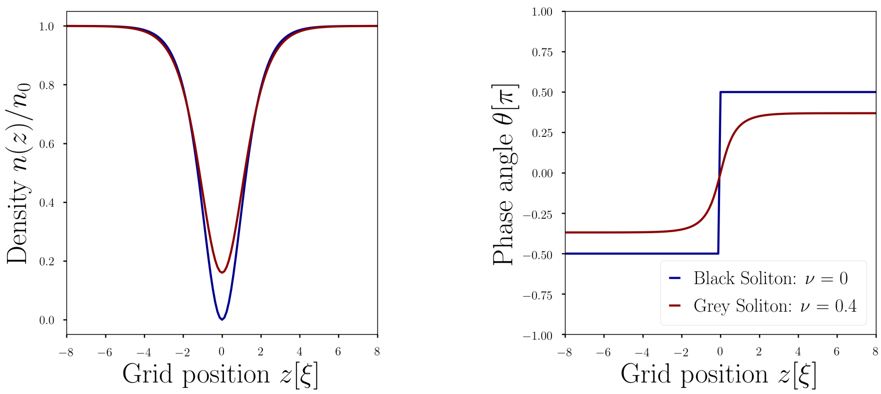


Figure 1: Density profile and phase of a single black and grey soliton

Solitons are localized density minima with a maximum density depression of ${}^{n_{\min}}/_{n} = \nu^2$, associated with a phase jump of $\Delta\theta \leq \pi$. They are called *black*, if $v_s = 0$ and *gray*, if $v_s \neq 0$. The physical momentum carried by the wave function due to the presence of the soliton is given by

$$p = m\int \mathrm{d}z\, j(z) = -2\hbar n\nu\sqrt{1-\nu^2} \tag{10}$$

with the current $j(z)$. It has a maximum at $\nu \approx 0.7$ [1].

1.4 Vortices

Another interesting excitation are vortices, which are a special property of superfluids. To get a better understanding of the density structure, we use cylindrical coordinates and evaluate the GPE for

$$\psi(\mathbf{r}) = f(n,z)\,\mathrm{e}^{il\varphi}\,. \tag{11}$$

This results in an additional term, i. e. ${}^{(\hbar l)^2}/_{2mn^2}$. which gives the kinetic energy resulting from its azimuthal velocity. The size of a typical vortex is about ξ. To visualize the density profile of a vortex we included a plot from [4].

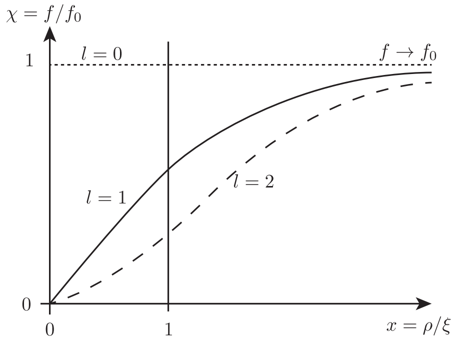


Figure 2: Density profile of a vortex, taken from [4]

Here, ρ is the background density, $l = 1, 2$ is the charge of the vortex and $l = 0$ is a situation without the presence of a vortex.
In this project, we are mainly interested in the evolution of different vortex constellations over time. This will be explained in more detail later on.
The final part of this introduction deals with the Split-Step Fourier method, our numerical approach for solving the GPE in this project.

1.5 The Split-Step Fourier method

The Split-Step Fourier method can be used to solve nonlinear partial differential equations. The result is obtained by evolving the system in both the time and the frequency domain. Therefore the differential equation is split into a linear and a nonlinear part, which can be considered/regarded separately by using sufficiently small steps. The transformation between time and frequency domain can be achieved efficiently by a fast Fourier transform (FFT) algorithm, which makes this method desirable.
In order to solve the GPE we first take a look at the time-dependent Schrödinger equation (3). In one spatial dimension its solution is

$$\psi(z, t + \Delta t) = \exp\left[\alpha\left(-\frac{\hbar^2}{2m}\nabla^2 + V(z)\right)\right]\psi(z, t). \tag{12}$$

We defined $\alpha := -\frac{i}{\hbar}\Delta t$ simply for convenience. Since the terms in the exponent do not commute, one cannot simply split the exponential function up. But if one rewrites the solution as

$$\psi(z, t + \Delta t) = \exp\left(\frac{\alpha}{2}V(z)\right) \cdot \exp\left(-\alpha\frac{\hbar^2}{2m}\nabla^2\right) \cdot \exp\left(\frac{\alpha}{2}V(z)\right) \cdot \psi(z, t), \tag{13}$$

the error is of $\mathcal{O}(\Delta t^3)$, which is accurate enough in our case and allows us to treat the two steps separately. Due to the fact, that V is diagonal in the time domain and ∇^2 is diagonal in the frequency domain, they simply become multiplications by $V(z)$ and the squared wavevector k^2, respectively. Combined with the speed of the FFT this enables a faster and more efficient way to obtain the result than calculating everything in the time domain would be. Putting everything together yields

$$\psi(z, t + \Delta t) = \exp\left(\frac{\alpha}{2}V(z)\right) \cdot \mathcal{F}^{-1}\left[\exp\left(-\frac{\alpha\hbar^2}{2m}k^2\right) \cdot \mathcal{F}\left[\exp\left(\frac{\alpha}{2}V(z)\right) \cdot \psi(z, t)\right]\right]. \tag{14}$$

Although we used the linear Schrödinger equation with time-independent Hamiltonian, the result is also true for the GPE if one replaces $V(x)$ by $V(x) + g\|\psi\|^2$. By using the

latest result in every step of the calculation one can ensure that the error does not exceed $\mathcal{O}(\Delta t^3)$.
Another important characteristic of the Split-Step Fourier method is, that it conserves the norm of the initial density distribution. To prove this for our implementation we normalized different initial constellations to 1 and plotted the norm after every time step during the evolution. The result is depicted in the following.

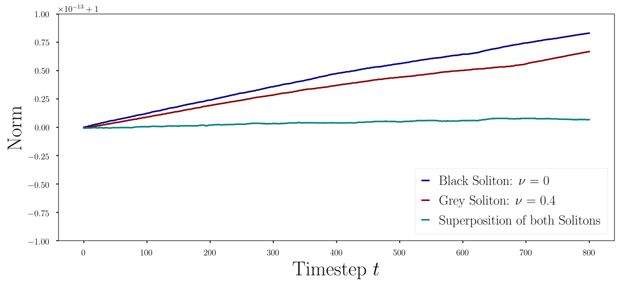


Figure 3: Proving the conservation of the norm by our implementation of the Split-Step Fourier method for different initial constellations.

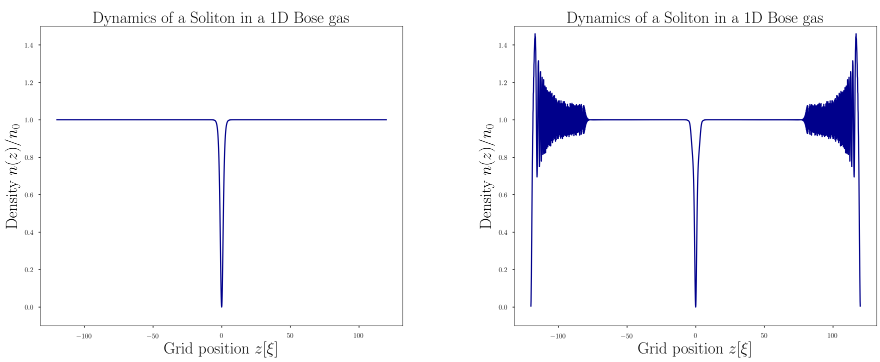
As one can see, for our implementation the norm ist conserved within a limit of $\mathcal{O}(10^{-13})$.

2 Evolution of dark solitons in a homogeneous 1D Bose gas

We start our analysis by initializing the density distribution on a spatial grid of length $L = 240$ with 2048 grid points, containing 2048 particles.
We took to analytic solution from equation (9) at $t = 0$ and used our implementation of the Split-Step Fourier method to determine its evolution, using a step size of $\mathrm{d}t = 0.01$. In total, we computed $N_{\text{steps}} = 800$ time steps. To discuss the results, we included some pictures of different time steps in the following. The animated evolution can be found in the corresponding Python notebook.

2.1 Single black soliton

We initialize a black soliton at $z_0 = 0$.

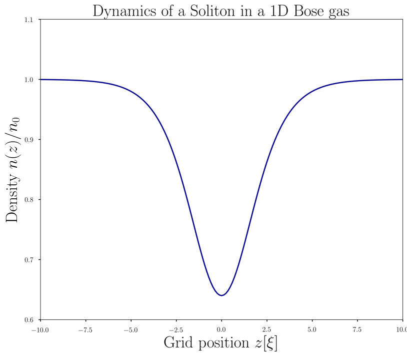


(a) Initial state **(b)** After $N_{\text{steps}} = 150$.

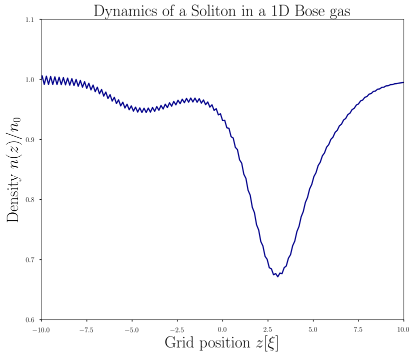
Figure 4: Dynamics of a single black soliton

2.2 Single grey soliton

We initialize a soliton with greyness $\nu = 0.8$ at $z_0 = 0$.



(a) Initial state

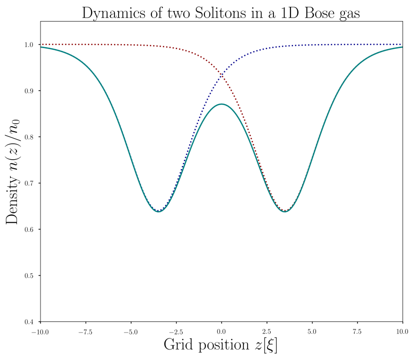


(b) After $N_{\text{steps}} = 400$.

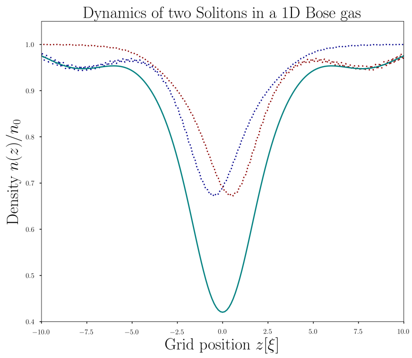
Figure 5: Dynamics of a single grey soliton

2.3 Two grey solitons moving in opposite directions

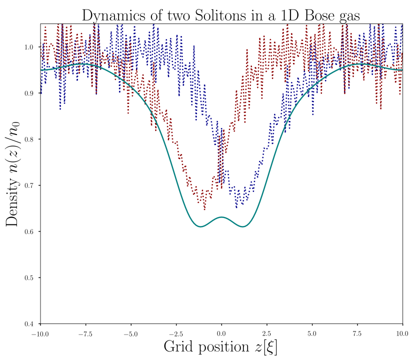
We initialize two solitons with greyness $\nu_1 = \nu_2 = 0.8$ at $z_{1,2} = \pm 3.5$.



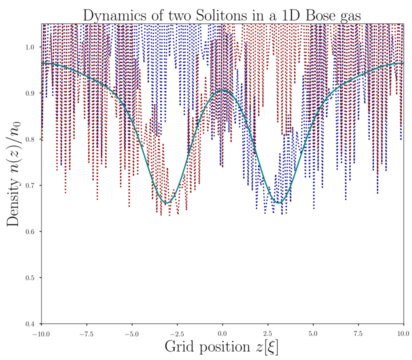
(a) Initial state



(b) After $N_{\text{steps}} = 400$.



(c) After $N_{\text{steps}} = 600$.



(d) After $N_{\text{steps}} = 800$.

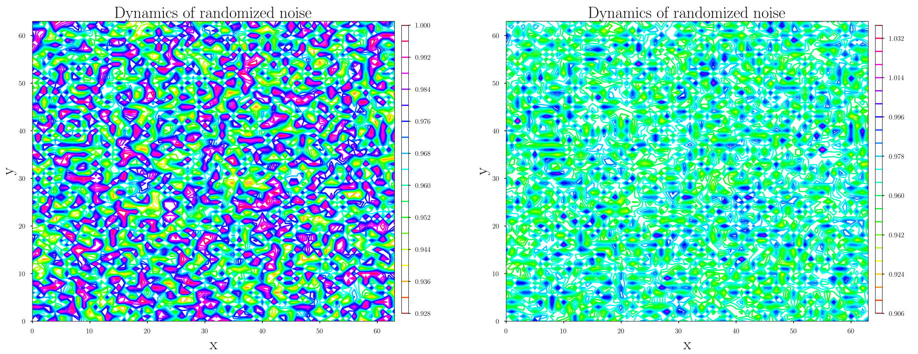
Figure 6: Dynamics of two grey solitons. The green line shows the superposition of both curves. It seems that the disturbing oscillations cancel each other out.

3 Evolution of perturbed density distributions in 2D

To perform calculations in two spatial dimensions, our initial grid and the Split-Step Fourier method have to be slightly modified. We use the given method to generate a homogenous density distribution. To study the dynamics of perturbations in two spatial dimensions, we analyze two different scenarios.
Our initial grid is now build up from 64×64 grid points and 4096 particles.
The animated evolutions can also be found in the corresponding Python notebook.

3.1 Randomized noise

We added some randomized noise of $\mathcal{O}(20\%)$ to the density distribution. Then we calculated the evolution of this perturbed distribution. Some pictures can be found in the following.

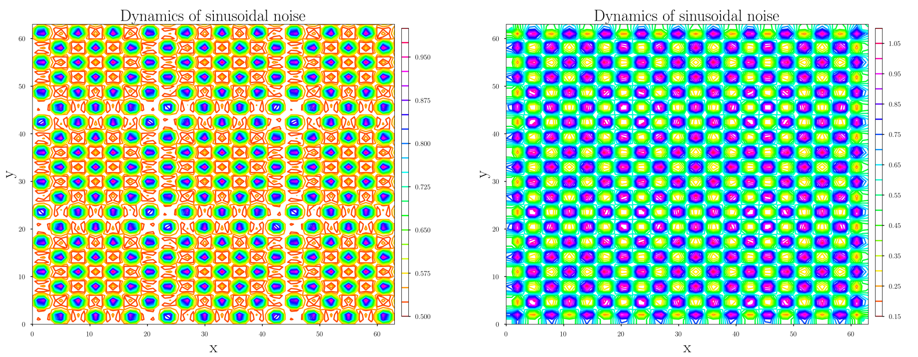


(a) Initial state **(b)** After $N_{\text{steps}} = 50$.

Figure 7: Evolution of a randomly perturbed density distribution

3.2 Sinusoidal noise

We initialized the grid with a small sinusoidal excitation.



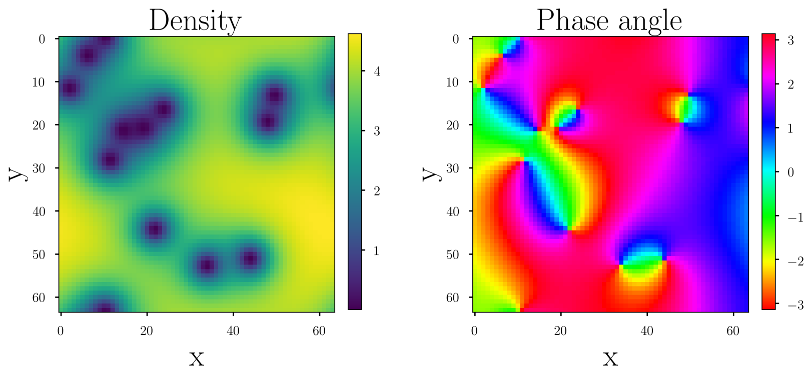
(a) Initial state **(b)** After $N_{\text{steps}} = 100$.

Figure 8: Evolution of a periodically perturbed density distribution

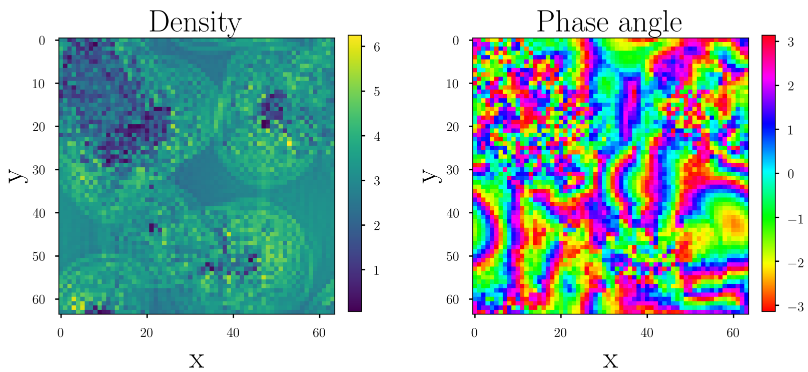
4 Visualizing the dynamics of vortices in a 2D Bose gas

The given routine creates vortices, differing in charge n, also known as winding number and arrangement. We try out some constellations including only single quantized vortices, vortex-antivortex pairs and vortices with higher charges. The evolution of the resulting densities and the corresponding phase distributions is depicted in the following.

4.1 Vortex-Antivortex pairs with the same charge



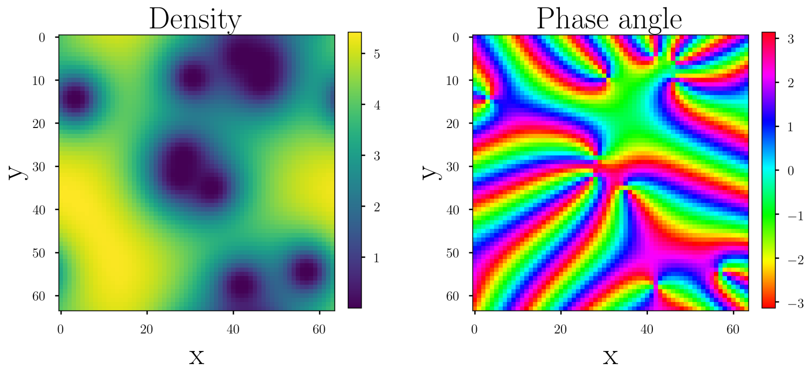
(a) Initial state



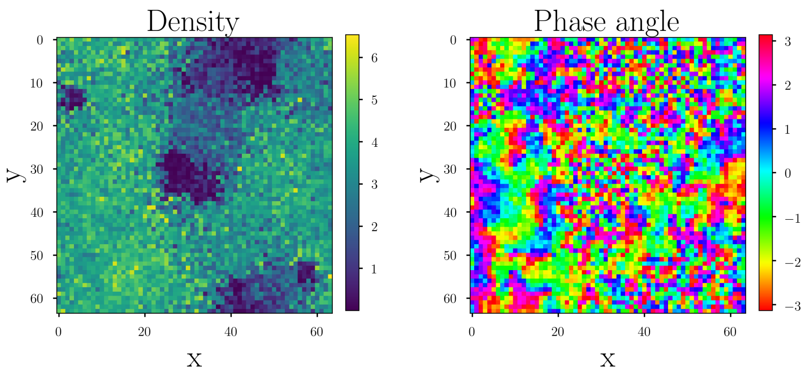
(b) After $N_{\text{steps}} = 50$.

Figure 9: Dynamics of vortex-antivortex pairs.

4.2 Randomly placed vortices with higher charges



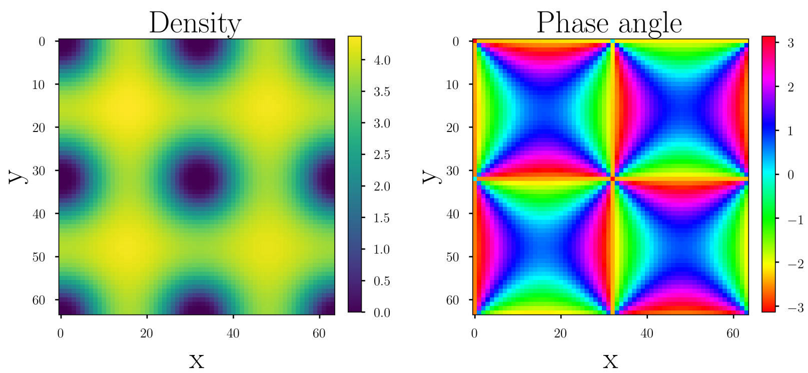
(a) Initial state



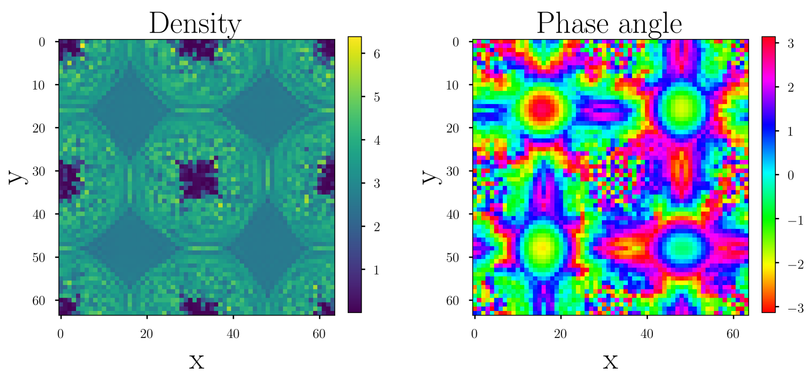
(a) After $N_{\text{steps}} = 80$.

Figure 11: Dynamics of a single black soliton

4.3 Equidistant placement of vortices with higher charges



(a) Initial state



(b) After $N_{\text{steps}} = 50$.

Figure 12: Dynamics of a single black soliton

5 Conclusion

In this section we want to conclude our results and compare them to what we would have expected.

Solitons in one spatial dimension We analyzed solitonic solutions of the GPE, discretized on a spatial grid. For the case of a black soliton with $\nu = 0$ we proved, that the distribution does not change over time. At the boundaries of the grid, we could observe some disturbing artefacts, which threaten the stability of our solution after long times.

For a single grey soliton with $\nu = 0.8$ we saw the expected movement in positive z-direction. Unfortunately the disturbing effects at the boundaries were a lot stronger in this case. Nevertheless we were able to reproduce the result one would expect from the analytical solution. The analytical time evolution is also included in the corresponding notebook.

In the case of two gray solitons, moving in opposite directions, we saw the overlapping in the center of the grid and after passing past each other the characteristic single movement, not effected by the collision.

Perturbed density distributions in two spatial dimensions We tried to perturb the two dimensional grid on two different ways, first by adding some randomized noise and second by adding a periodic, sinusoidal noise structure. Both distributions showed interesting dynamics over time. The randomized noise seams to vanish after long times, i. e. the distribution get's smoother. This was not what we expected intuitively at the beginning , but after playing around with the vortex grids in the third part, it seems that the artificially added defects are not stable at all. The second example showed the same long-term behavior.

Vortices as topological defects

References

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